Sacharidy a lipidy
Glykobioinformatika a lipidoinformatika

C2131 Úvod do bioinformatiky, jaro 2023

Lenka Malinovská

Cukry

4.7.5 carbohydrate (saccharide)

Monosaccharides, *oligosaccharides* and *polysaccharides*, as well as substances derived from monosaccharides by reduction of the carbonyl group (alditols), by oxidation, including the oxidation of one or more terminal groups to carboxylic acids, or by replacement of one or more hydroxy groups by a hydrogen atom, an amino group, a thiol group, or by similar heteroatomic groups. This term also includes derivatives of these compounds.

Note: The term carbohydrate was applied originally to monosaccharides, in recognition of the fact that their empirical composition can be expressed as $C_m(H_2O)_n$. However, the term is now used generically in a wider sense.

4.7.35 monosaccharide

Polyhydroxy aldehyde H-[CHOH]$_n$-CHO or polyhydroxy ketone H-[CHOH]$_n$-CO-[CHOH]$_m$-H, with at least three or more carbon atoms, respectively.

Note 1: The generic term monosaccharide (as opposed to *oligosaccharide* or *polysaccharide*) denotes a single unit without glycosidic connection to other such units.

Note 2: Most monosaccharides exist as cyclic *hemiacetals* or *hemiketals*.

Examples: *Aldoses*, dialdoses, aldoketoses, *ketoses*, diketoses, as well as deoxy sugars and amino sugars, and their derivatives, provided that the compound has a (potential) carbonyl group.

4.7.37 oligosaccharide

Compound in which *monosaccharide* units are joined by *glycosidic linkages*.

Note: Oligosaccharides are called disaccharides, trisaccharides, tetrasaccharides, pentasaccharides, *etc.*, according to their number of units.

4.7.38 polysaccharide

Biomacromolecule consisting of a large number of *monosaccharide* (glycose) residues joined to each other by *glycosidic linkages*.

See *glycan*

Carbohydrate (saccharide) = cukr, sacharid = obecný termín pro celou skupinu látek

Glykan = složitější cukr, oligosacharid nebo polysacharid, volný nebo vázaný

V oboru chemie potravin jsou výrazem cukry označovány pouze monosacharidy a oligosacharidy. Dle legislativy jsou jako cukry označovány monosacharidy a disacharidy.

POZOR! POUŽITÍ JEDNOTLIVÝCH TERMÍNŮ SE TEDY LIŠÍ DLE VĚDNÍHO OBORU!

Terminology of bioanalytical methods (IUPAC Recommendations 2018)

https://doi.org/10.1515/pac-2016-1120
Received November 21, 2016; accepted February 1, 2018

Cukry

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HLAVNÍ ŽIVINY

- Bílkoviny
- Lipidy (tuky)
- **Sacharidy**
  - množstvím ve stravě (55-60% celkového energetického příjmu) představují její základní složku
  - poskytují organizmu energii
  - jiný biologický význam je nepatrný

www.vyzivaspol.cz

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Funkce cukrů

Zdroj energie

Sacharosa, glukosa,...

Nosič informace

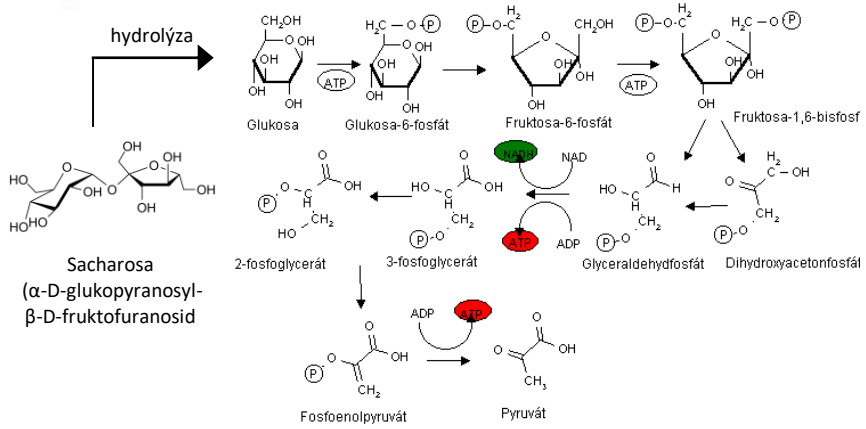
Krevní skupiny,...

Strukturní role

Celulosa, chitin...

Funkce cukrů

Zdroj energie

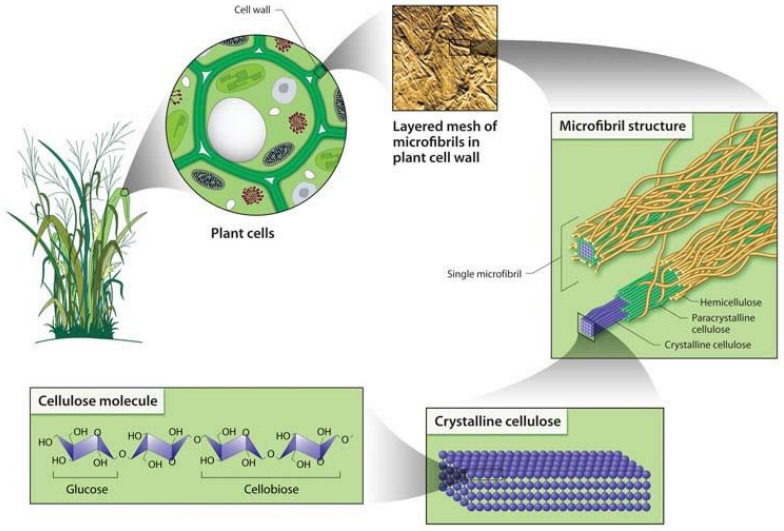


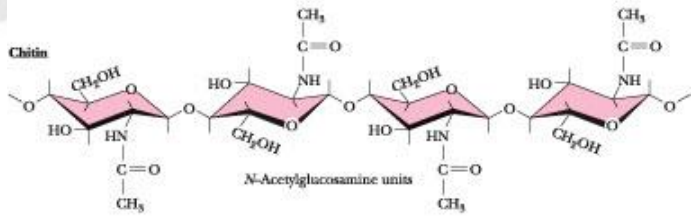
Sacharosa
(α-D-glukopyranosyl-
β-D-fruktofuranosid

Nosič informace

Krevní skupiny,...

Strukturní role

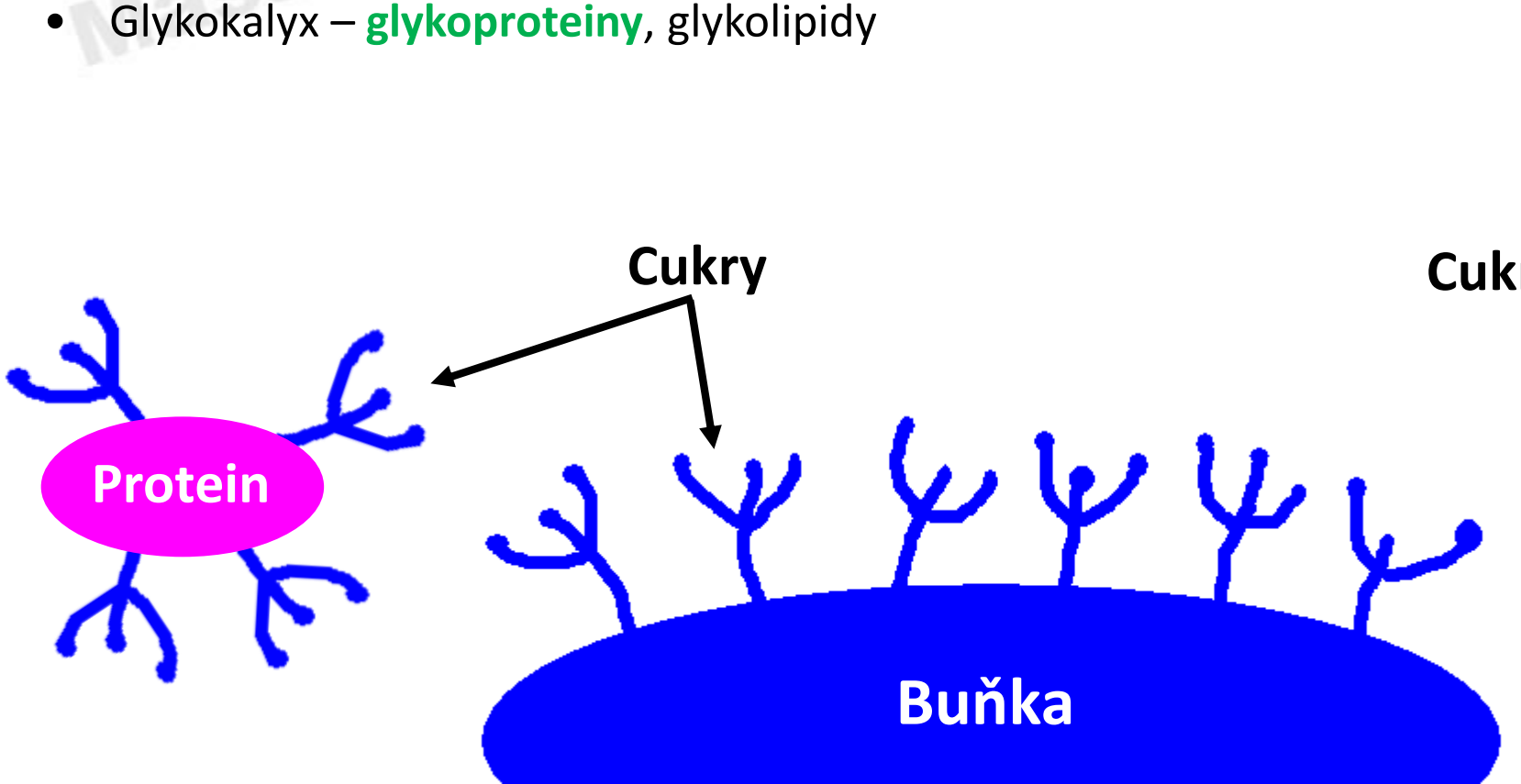


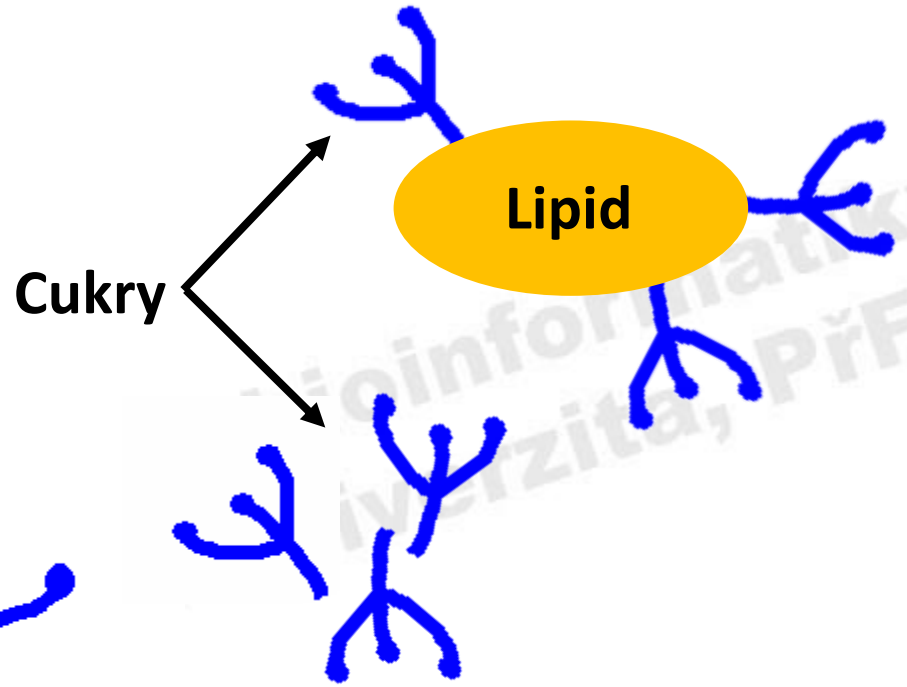


Výskyt cukrů v buňce

- Jádro – součást **nukleových** kyselin (ribosa, deoxyribosa)
- Cytosol – volné monosacharidy
- Endoplasmatické retikulum, Golgiho aparát – glykosylované proteiny
- Buněčná stěna – vázané oligo a polysacharidy
- Glykokalyx – **glykoproteiny**, glykolipidy

- **Glykom** – soubor všech sacharidů produkovaných organismem (buňkou, tkání) v daném čase za daných podmínek.

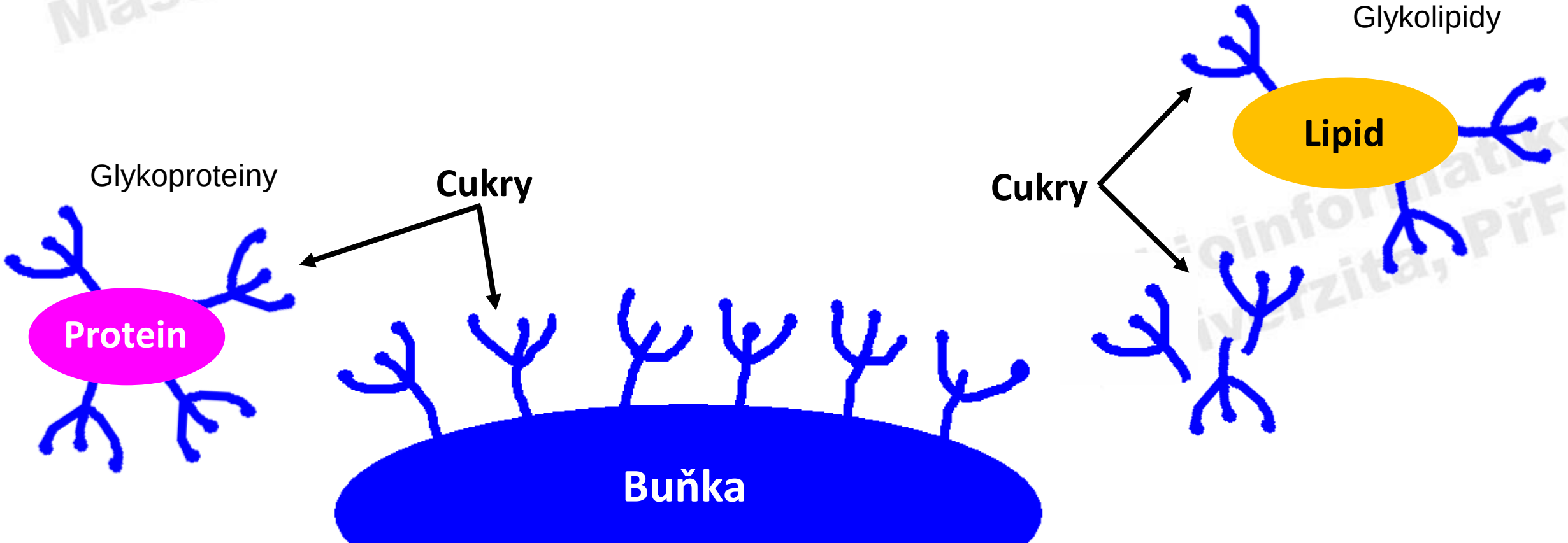




Výskyt cukrů v buňce

- Kovalentně vázané cukry (monosacharidy, oligosacharidy) se nacházejí na povrchu všech buněk.
- Jsou součástí mnoha makromolekul.
- Mohou se v buňce nacházet i samostatně.

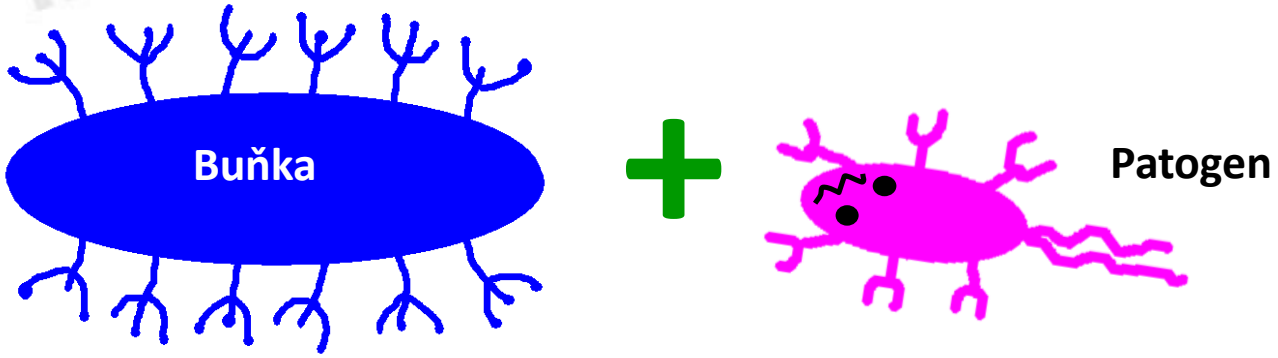
- **Protože se nacházejí na povrchu buněk a makromolekul, mohou se cukry uplatňovat v komunikaci a interakcích mezi buňkami a molekulami.**

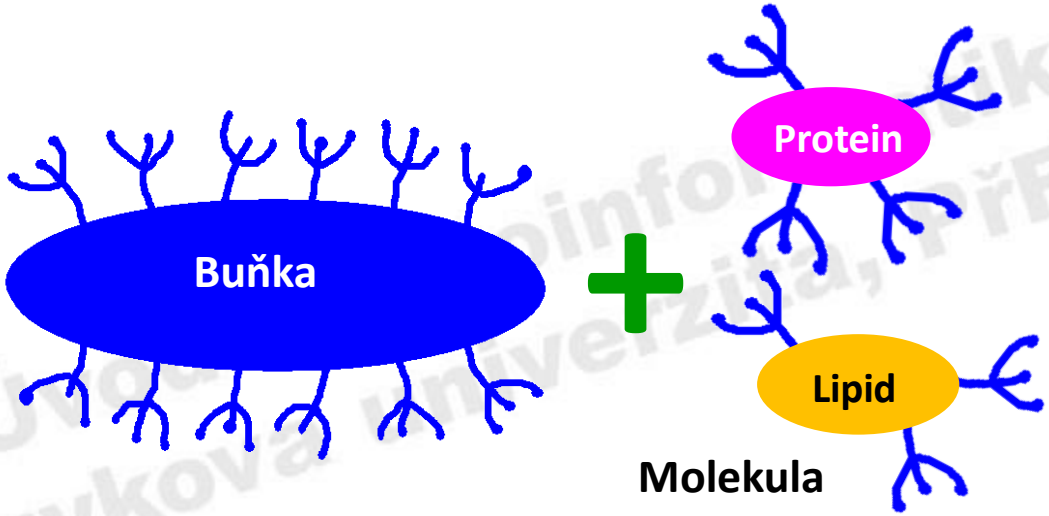


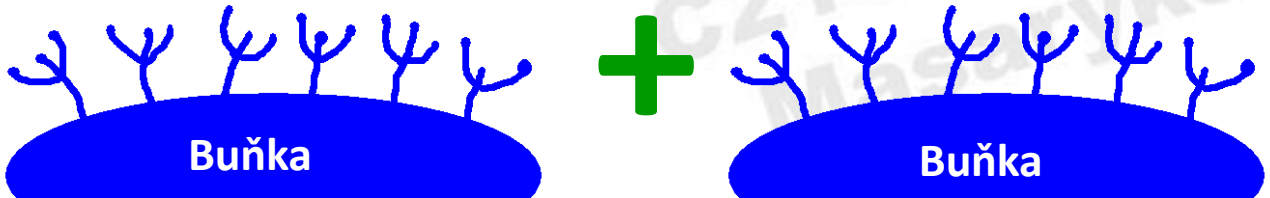
Výskyt cukrů v buňce

- Interakce buňka-buňka
- Interakce buňka-molekula
- Interakce buňka-patogen

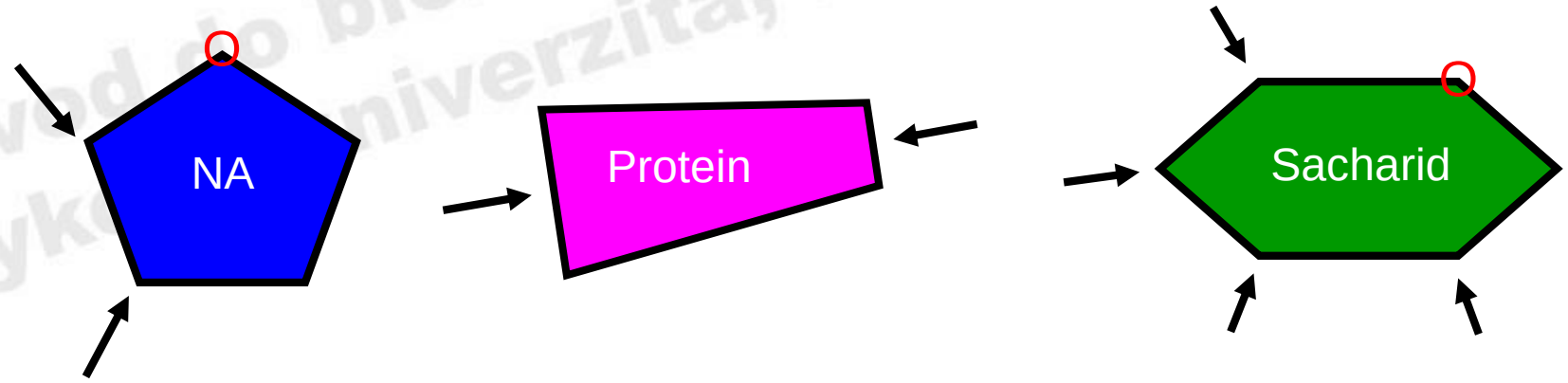
- **Protože se nacházejí na povrchu buněk a makromolekul, mohou se cukry uplatňovat v komunikaci a interakcích mezi buňkami a molekulami.**







Informační potenciál biomolekul

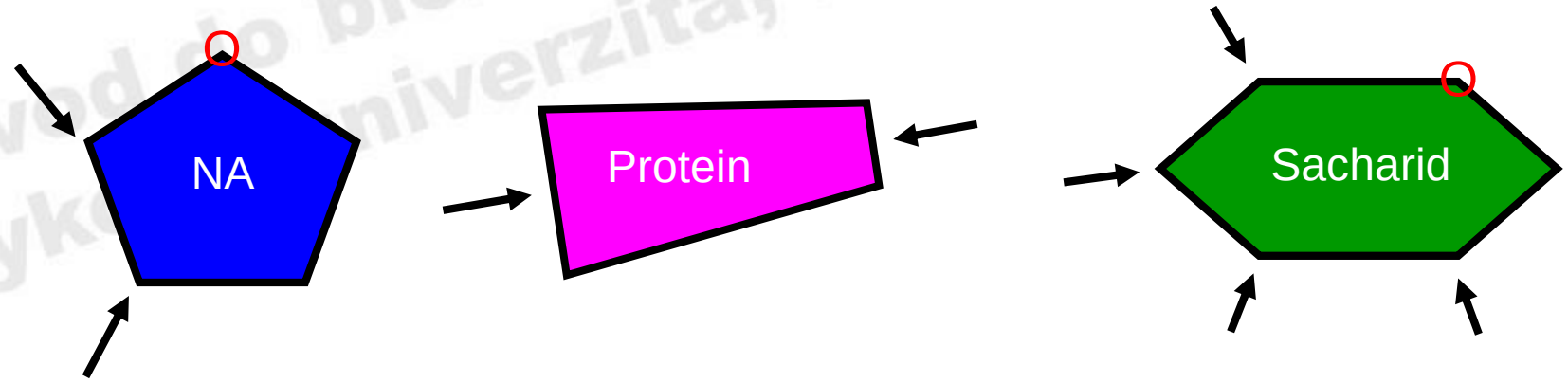


- Informační potenciál je určen množstvím „slov“ (isomerů), které je možné sestavit z jednotlivých „písmen“ (monomerů).
- Nukleotidy a aminokyseliny vytvářejí **lineární polymery**, spojované stále stejným způsobem (fosfodiesterová vazba, peptidová vazba).
- K dokonalému popisu obsažené informace stačí pouze **jednoduchá sekvence** (sled) monomerů:

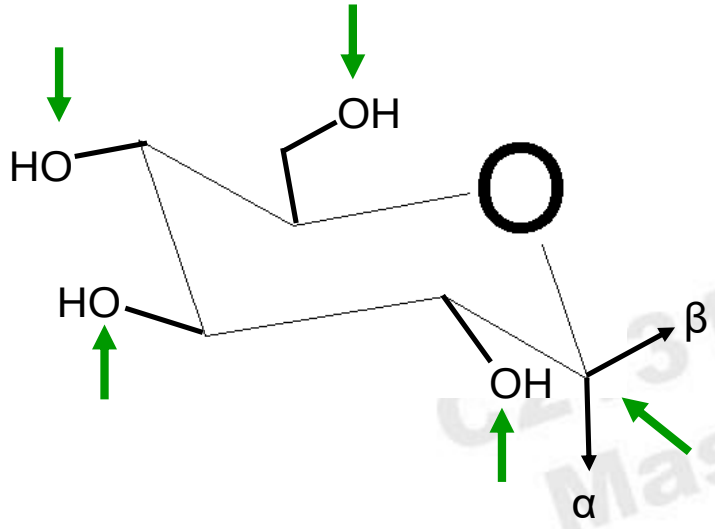
ATGCTGGTGATTGTGGATGCCGTTACCCTGCTGAGCGCCTATCCGGAAGCCAGCCGTGATC
CGGCCGCCCCGACCGTGATTGATGGTCGCCACCTGTATGTTGTTAGCCCGGGCGATGCCGC

MLVIVDAVTLLSAYPEASRDPAAPTVIDGRHLYVVSPGDA

Informační potenciál cukrů



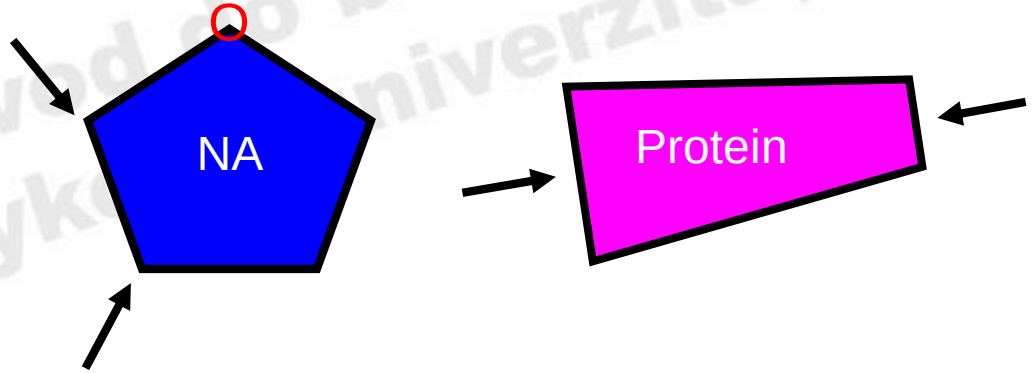
- Pro přesný popis oligo(poly)sacharidu je kromě sekvence nutné znát i typ glykosidické vazby (anomerii) a velikost kruhu.



D-glukosa + D-glukosa:

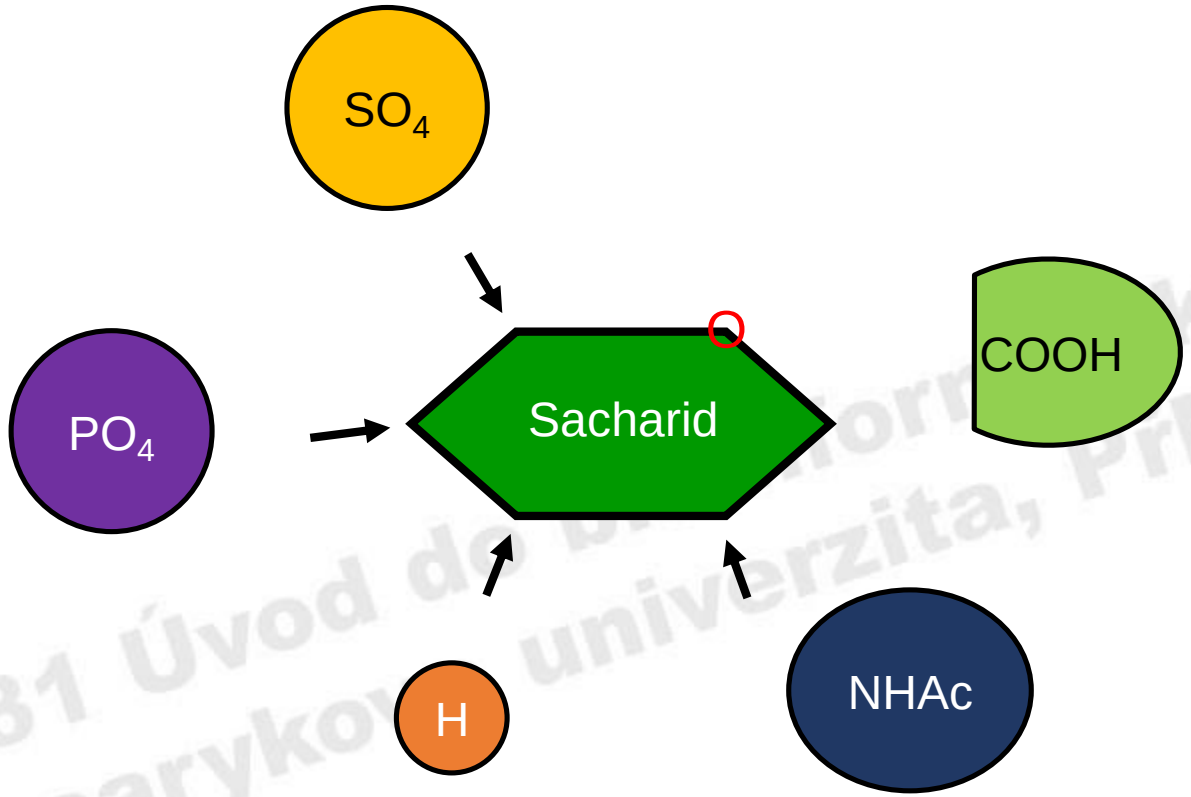
α1-2	**kojibiosa**
α1-3	**nigerosa**
α1-4	**maltosa**
α1-6	**isomaltosa**
α1-1´α	**trehalosa**
β1-2	**soforosa**
β1-3	**laminaribiosa**
β1-4	**cellobiosa**
β1-6	**gentibiosa**

Informační potenciál cukrů



- Glykosidické vazby může tvořit i více než jedna OH skupina, vzniká **rozvětvený** oligosacharid.
- Klasickým příkladem rozvětvených oligosacharidů jsou antigeny **AB0 krevních skupin.**

- Cukry mohou být dále **modifikovány** redukcí, oxidací nebo vazbou dalších funkčních skupin.



„Cukerný kód“

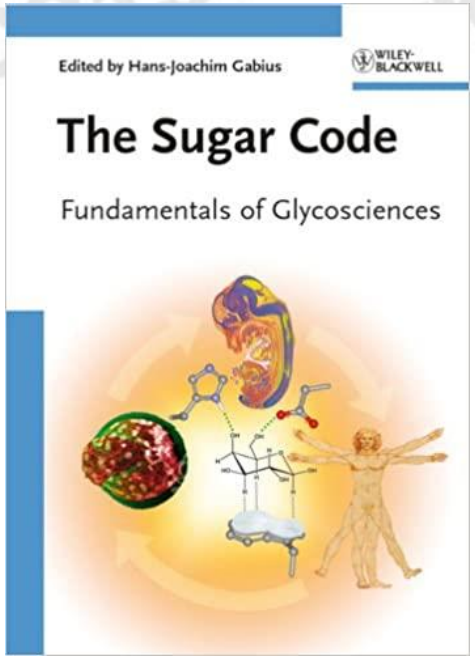
Evolutionary aspects of ABO blood group in humans

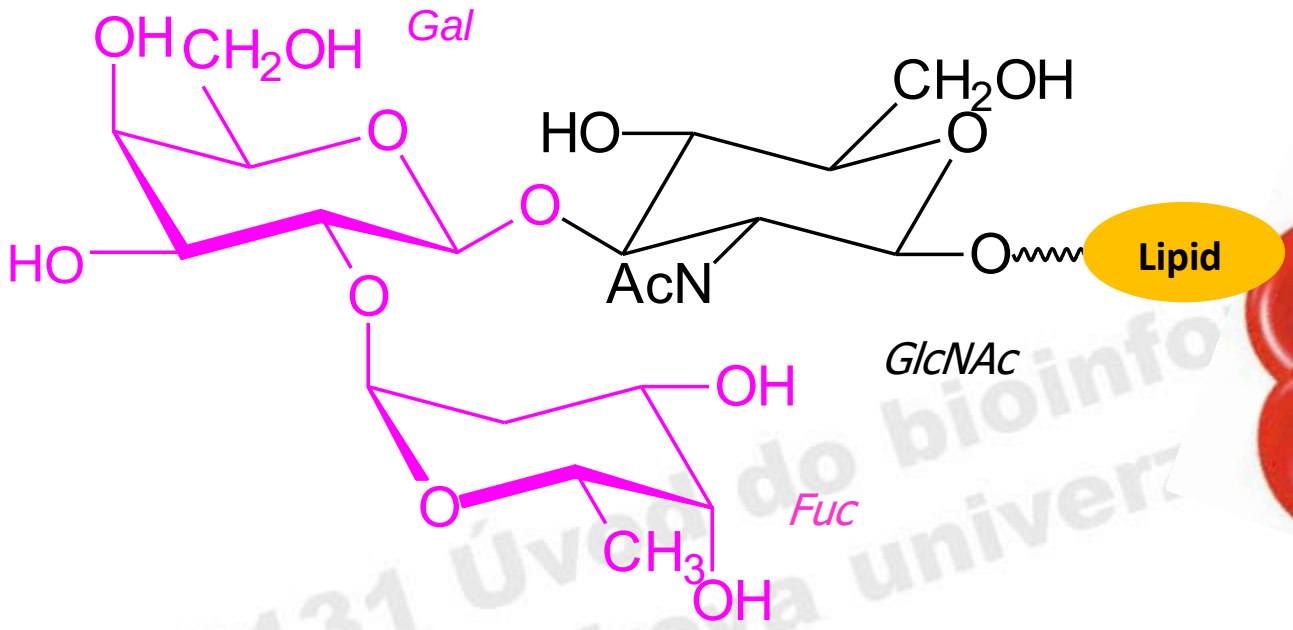
Massimo Franchini *, Carlo Bonfanti

Department of Hematology and Transfusion Medicine, Azienda Ospedaliera Carlo Poma, Mantova, Italy

ABSTRACT

The antigens of the ABO blood group system (A, B and H determinants) are complex carbohydrate molecules expressed on red blood cells and on a variety of other cell lines and tissues. Growing evidence is accumulating that ABO antigens, beyond their key role in transfusion medicine, may interplay with the pathogenesis of many human disorders, including infectious, cardiovascular and neoplastic diseases. In this narrative review, after succinct description of the current knowledge on the association between ABO blood groups and the most severe diseases, we aim to elucidate the particularly intriguing issue of the possible role of ABO system in successful aging. In particular, focus will be placed on studies evaluating the ABO phenotype in centenarians, the best human model of longevity.





Tkáňové a krevní skupiny AB0

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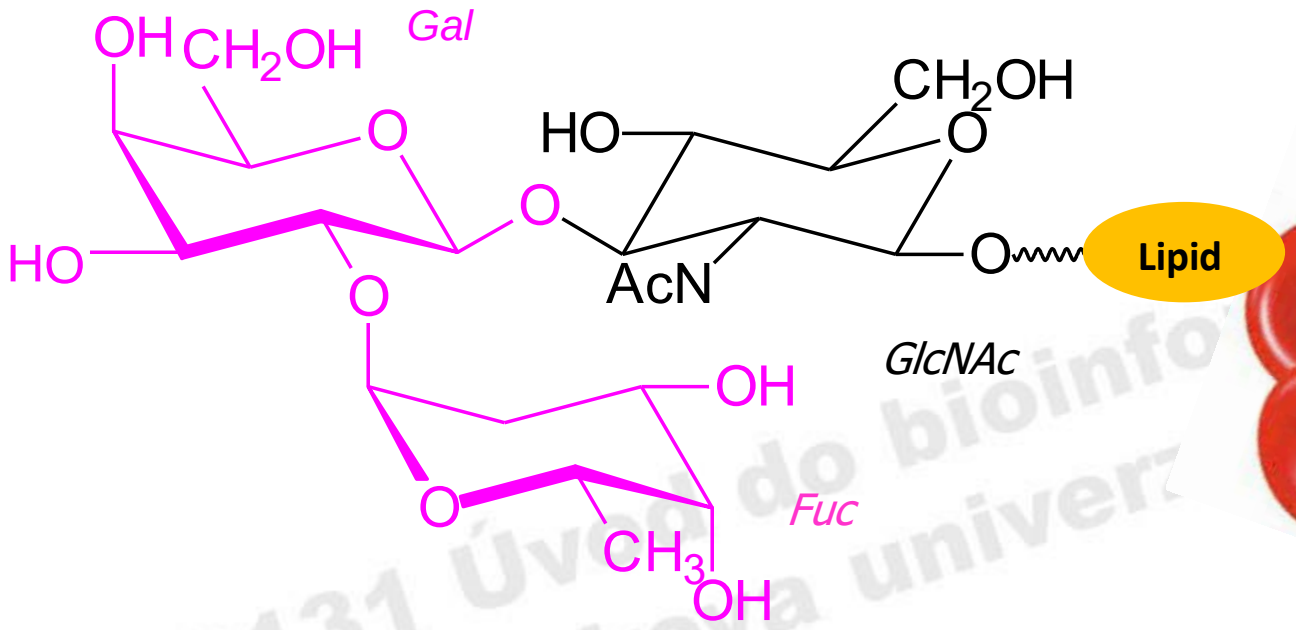

Krevní skupina 0

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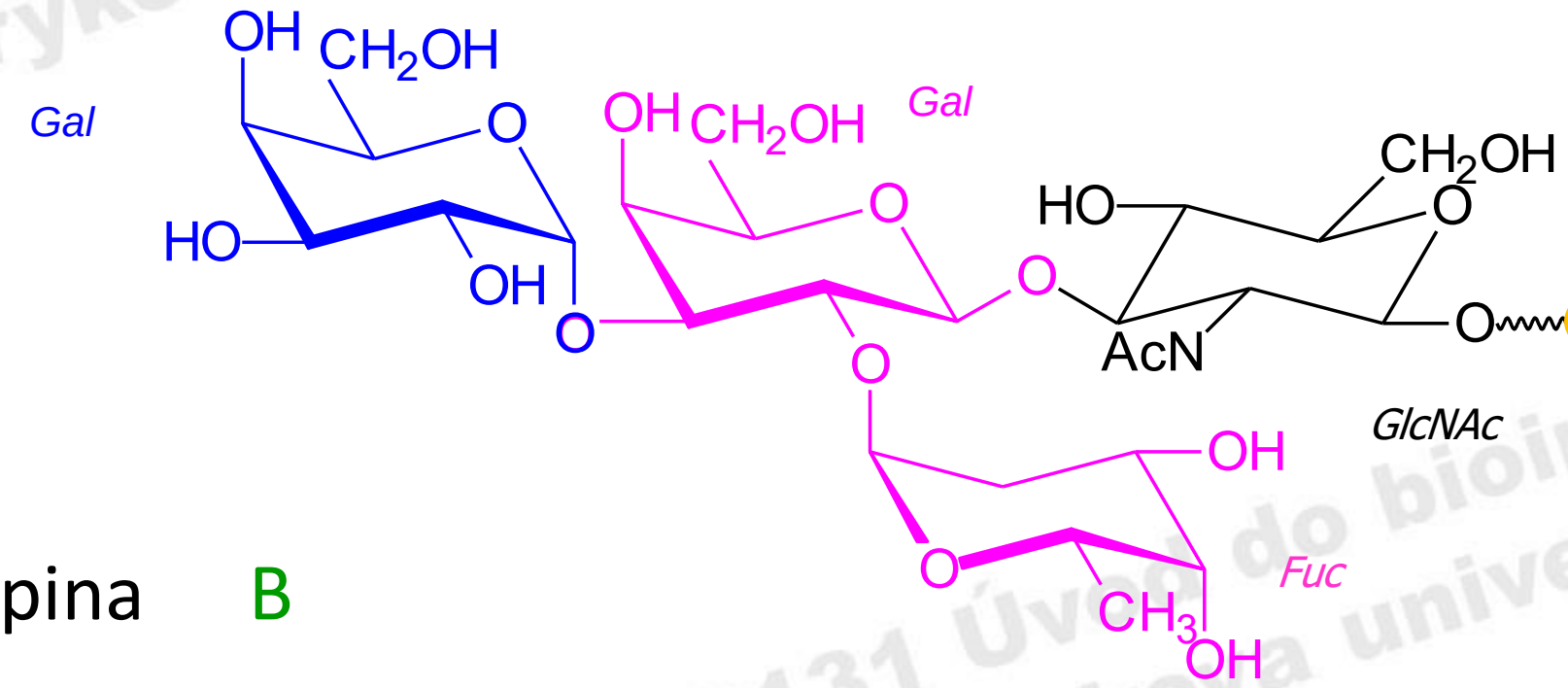

Krevní skupina B

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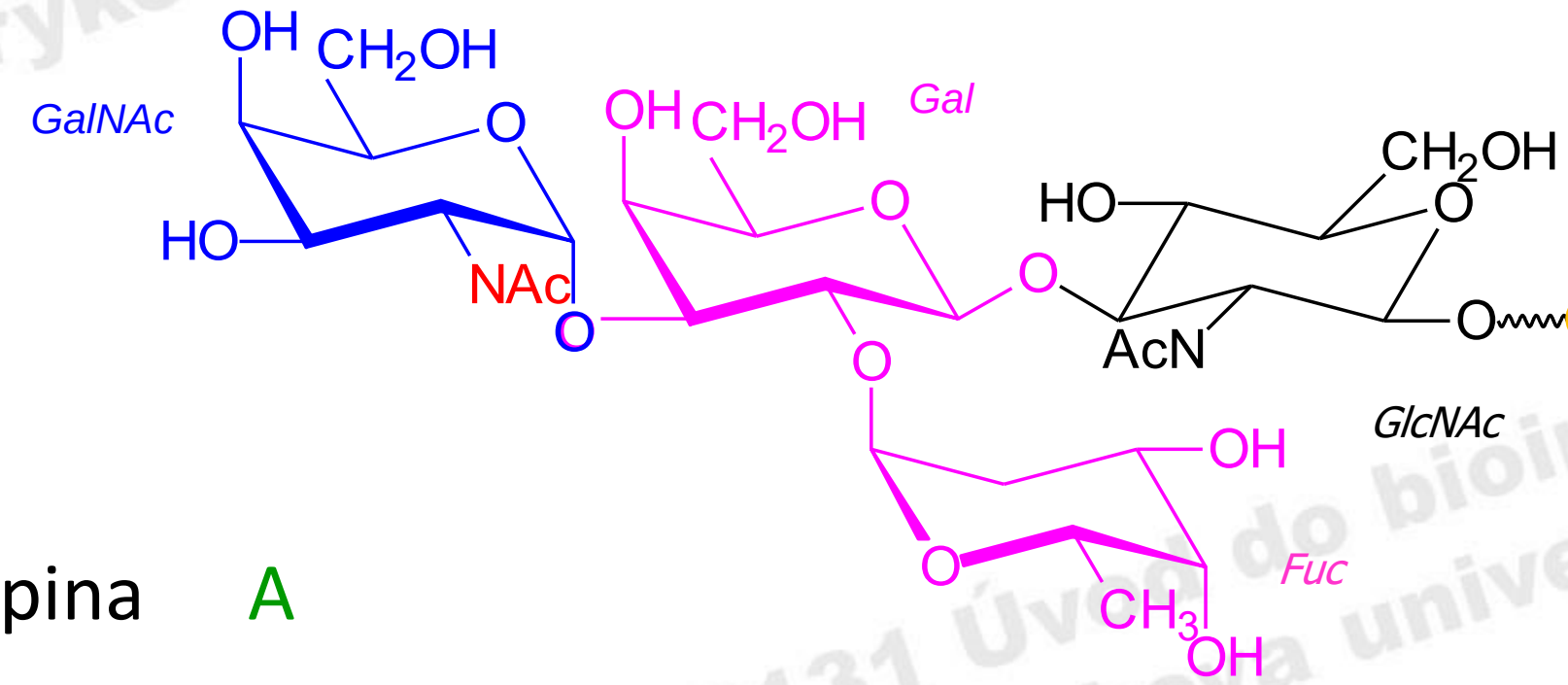


Krevní skupina A

Tkáňové a krevní skupiny AB0

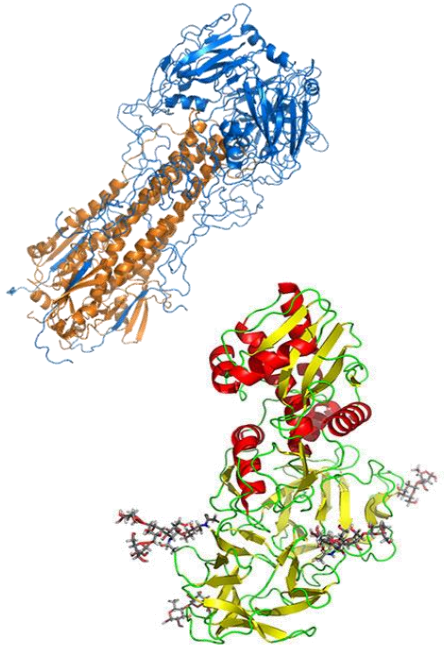
Čtení „cukerného kódu“

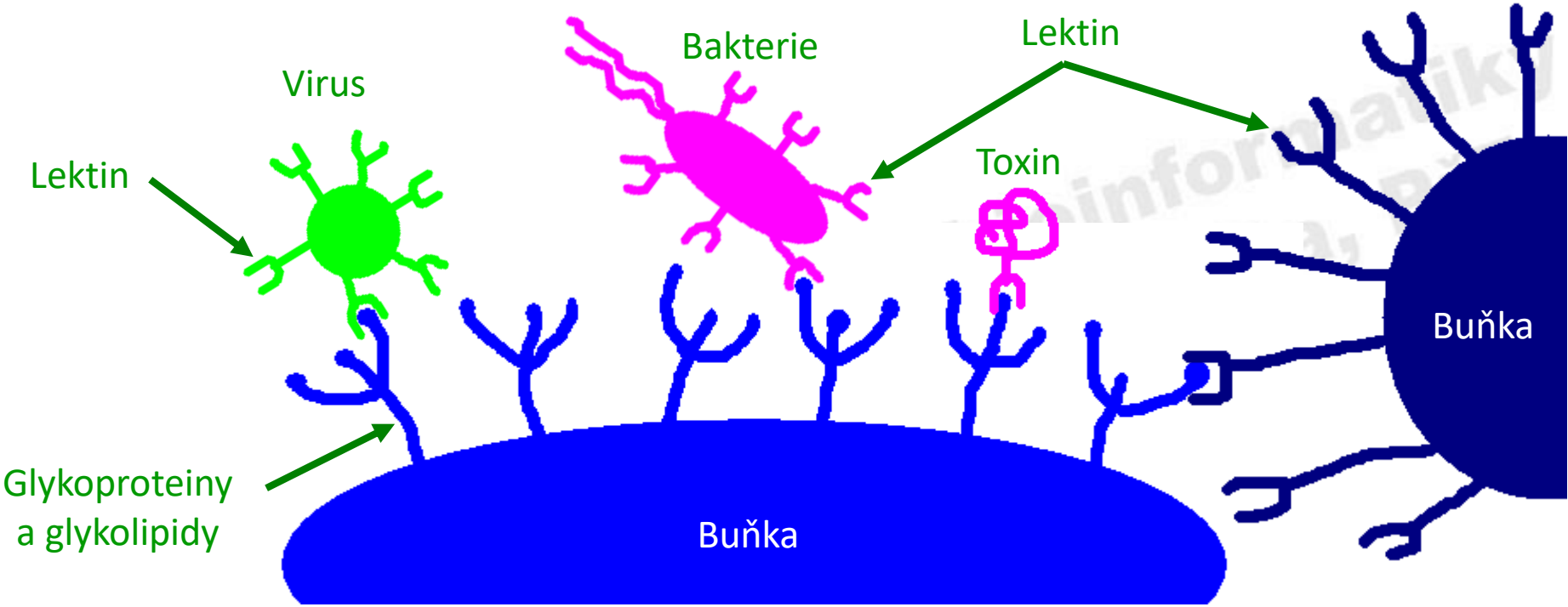

Lectins

Nathan Sharon, Weizmann Institute of Science, Rehovot, Israel

Based in large part on the previous version of this Encyclopedia of Life Sciences (ELS) article, Lectins by Nathan Sharon and Halina Lis.

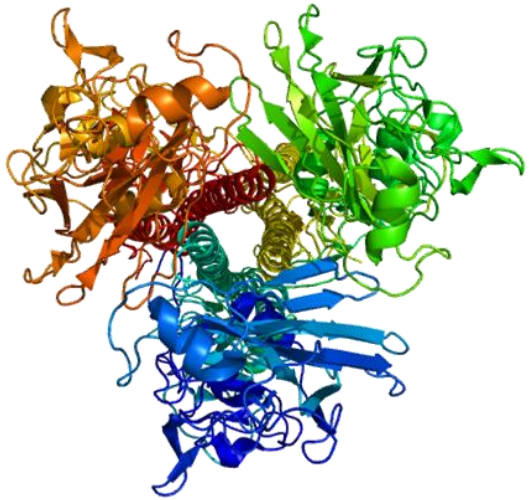
- **Protilátky**
- **Lektiny** – proteiny, které specificky a reverzibilně vážou mono- a oligosacharidy. Nejsou produkty imunitní odpovědi.
- Lektiny plní rozpoznávací a adhezivní funkci v mnoha různých biologických procesech.
- Vyskytují se v zástupcích všech taxonů (rostliny, zvířata, houby, bakterie, viry).

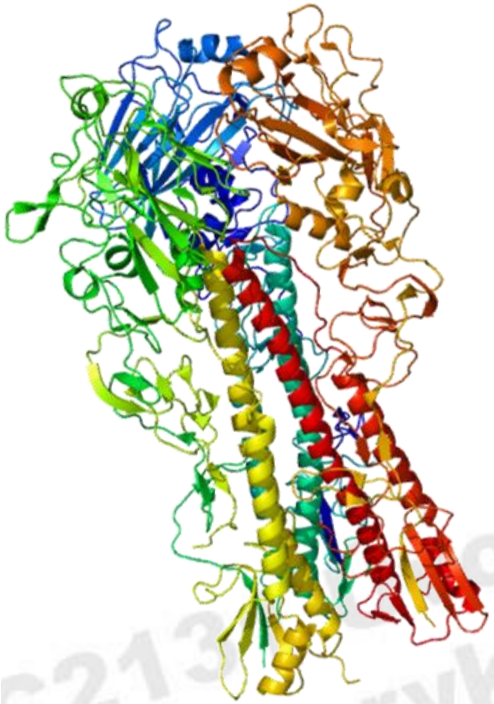




Hemaglutinin viru chřipky

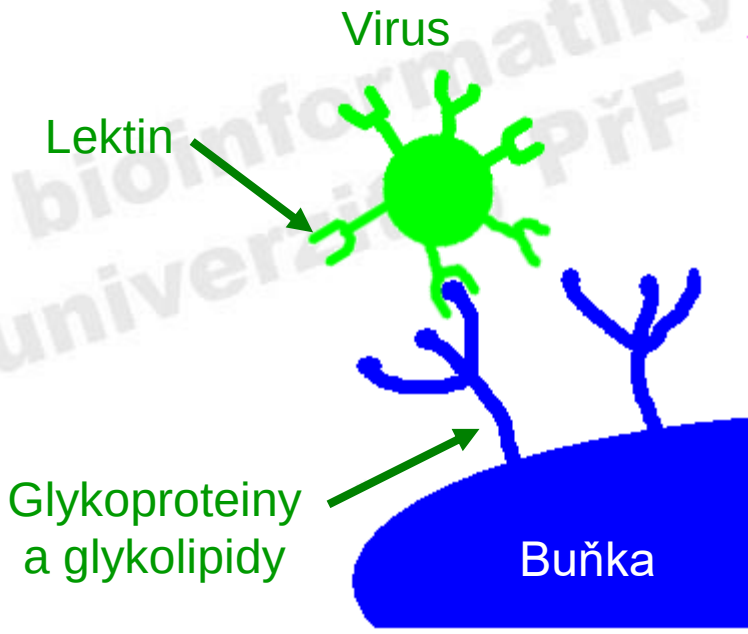
- Virus chřipky A obsahuje povrchový glykoprotein, **hemaglutinin** (HA). Tento protein je lektin, který rozpoznává hostitelské buňky a řídí adhezi a vstup viru do buněk.





New insights into influenza A specificity: an evolution of paradigms

Ye Ji, Yohanna JB White, Jodi A Hadden[1], Oliver C Grant and Robert J Woods



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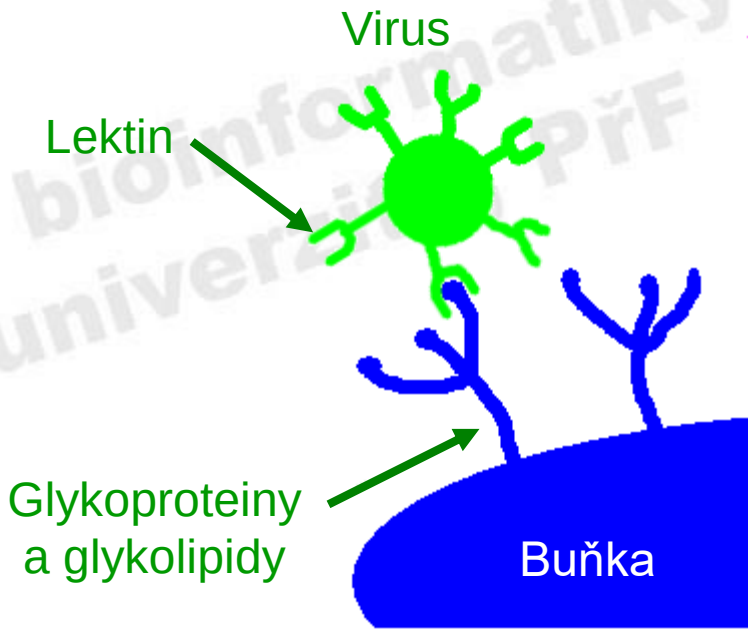
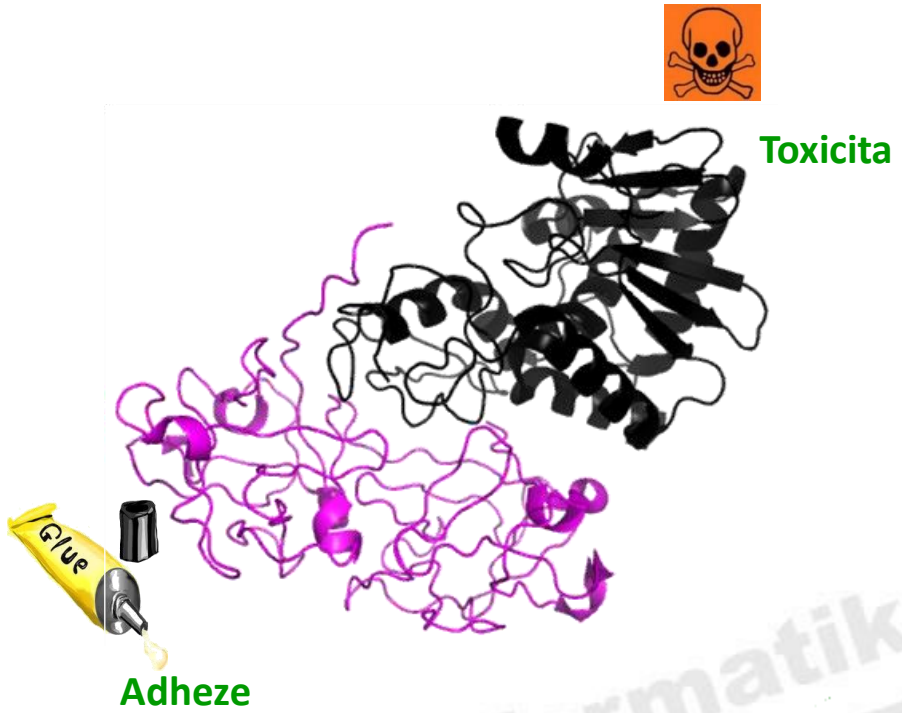
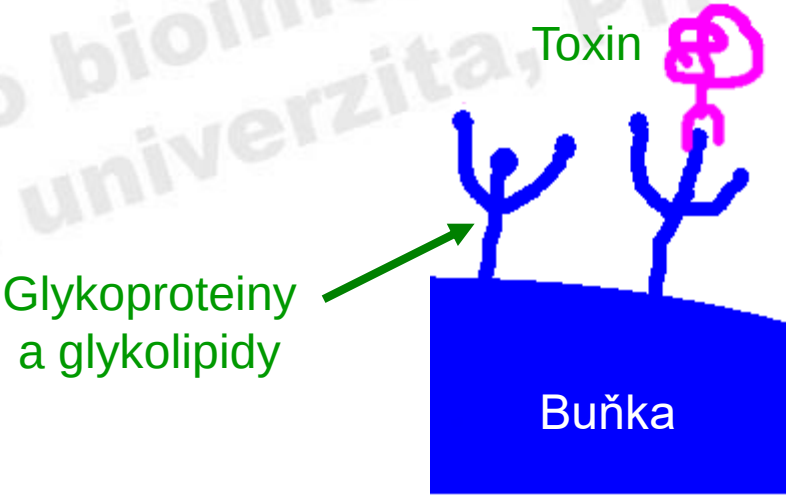


Ricin

- **Ricin** je toxin produkovaný rostlinou *Ricinus communis* (skočec obecný, Ricín obyčajný).
- Často využíván jako **okrasná rostlina**.
- Ricin se vyskytuje nejvíce v **semenech**.
- Pro otrávení jsou celá semena nevhodná, je nutné je pořádně rozžvýkat.



Ribosome-inactivating proteins (RIPs) – proteiny inaktivující ribosomy
Ricin, abrin, volkensin



Ricin

Tajné služby zadržely otrávený dopis pro Obamu. Obsahoval jed ricin

17. dubna 2013 18:06, aktualizováno 21:07

Americké tajné služby zajistily v úterý dopis adresovaný prezidentu Baracku Obamovi, který obsahoval podezřelou látku. Dopis byl zachycen v objektu, který leží mimo komplex Bílého domu. Podle prvních testů federální policie obsahoval jedovatý ricin.

Americkému senátorovi poslali dopis s ricinem

Dopis zaslaný republikánskému senátorovi za stát Mississippi Rogeru Wickerovi obsahoval ricin. Potvrdil to předběžný test, jsou ale ještě potřeba další zkoumání. List se podařilo zachytit ještě v oddělení, které pro zákonodárce poštu zpracovává. O nálezu informoval šéf policie v Capitolu Kim Dine s tím, že případ převzal Federální úřad pro vyšetřování (FBI).

Newyorskému starostovi poslali dopis s ricinem

Dopisy adresované newyorskému starostovi Michaelu Bloombergovi a organizaci podporující omezení prodeje zbraní, obsahovaly jedovatý ricin, uvedly úřady po testech. Jeden z bezpečnostních pracovníků, který přišel s dopisem do styku, vykazuje drobné příznaky kontaktu s ricinem.

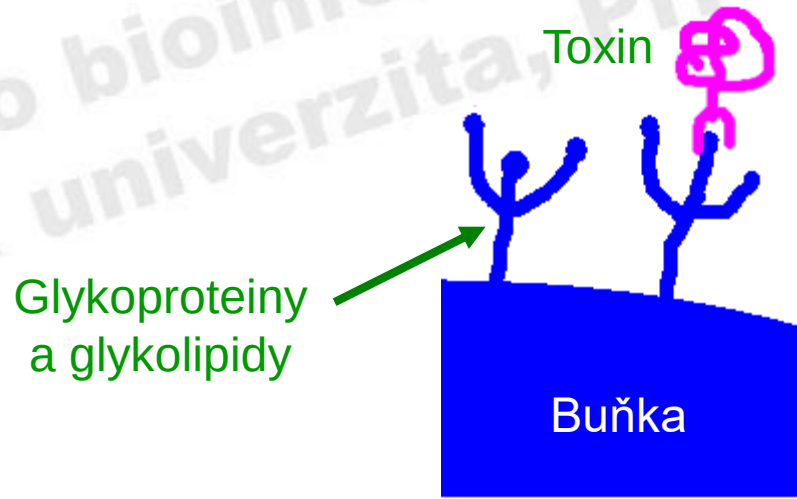
Deštníková vražda bulharského spisovatele Markova

Toto jméno je neustále s námi…

7. 9. 2008

Londýn - Do dějin případ vstoupil jako „deštníková vražda“ a dodnes není objasněn. Neznámý pachatel vpravil 7. září 1978 v Londýně pomocí speciálně upraveného deštníku jed do těla bulharského spisovatele a disidenta Georgiho Markova, který za čtyři dny zemřel. Podezření padlo na bulharskou komunistickou tajnou službu a kdysi obávanou sovětskou tajnou policii KGB. Podle některých spekulací si zabití Markova, který v Londýně pracoval v bulharské sekci rozhlasové stanice BBC, objednal osobně vůdce bulharských komunistů Todor Živkov, protože Markov, kdysi prominentní spisovatel a později ostrý kritik poměrů v Bulharsku, toho příliš mnoho věděl o životě bulharských vládců. Zajímavostí je, že Živkov slavil právě 7. září 1978 sedmašedesátiny.

https://ct24.ceskatelevize.cz/archiv/1442570-destnikova-vrazda-bulharskeho-spisovatele-markova



Ricin není jed, ale projímadlo. Zemanovy výroky vyvolaly kritiku

6. května 2020 16:28

Prezident Miloš Zeman vyvolal značnou kritiku mezi politiky, když v úterý popřel přítomnost ruského agenta v Praze a zkritizoval dvě zpravodajské služby. Řadu lidí popudil i tím, že ricin označil za projímadlo.

Agent s ricinem pobouřil diplomacii. Radikální kroky nejsou třeba, říká Babiš

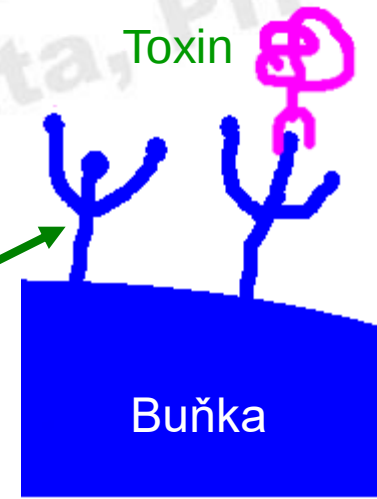
28. dubna 2020 16:51, aktualizováno 20:51

Rusko popřelo informace týdeníku Respekt, že do Prahy dorazil agent tamních tajných služeb s jedem ricinem, kterého bezpečnostní úřady vyhodnotily jako riziko pro politiky Ondřeje Koláře a Zdeňka Hřiba. Rusko zprávu časopisu označilo za novinářskou „kachnu“, to však česká diplomacie považuje za snahu o narušování svobody tisku. Senát žádá vládu, aby ohledně chování Ruska zakročila, podle premiéra Babiše ale nejsou potřeba radikální kroky.

Newyorskému starostovi poslali dopis s ricinem

„Snad jeden z nejznámějších léčebných použití ricinového oleje je jako přírodní projímadlo. Je klasifikován jako stimulační projímadlo, což znamená, že zvyšuje pohyb svalů, které vytlačují materiál skrz střeva, a pomáhá tak vyčistit střeva. Stimulační laxativa působí rychle a běžně se užívají ke zmírnění dočasné zácpy.“

To si pan prezident plete s ricinovým olejem. Ricinový olej se vyrábí z těch stejných semen *R. communis*, která obsahují ricin. Ricinu se ale do olejové fáze moc nechce a olej je navíc ohříván, takže ricin (protein) je bezpečně denaturován. Ricin by pochopitelně skutečně fungoval jako projímadlo…taky je to emetikum a snižuje krevní tlak. Někdy až na nulu.



Chem Soc Rev

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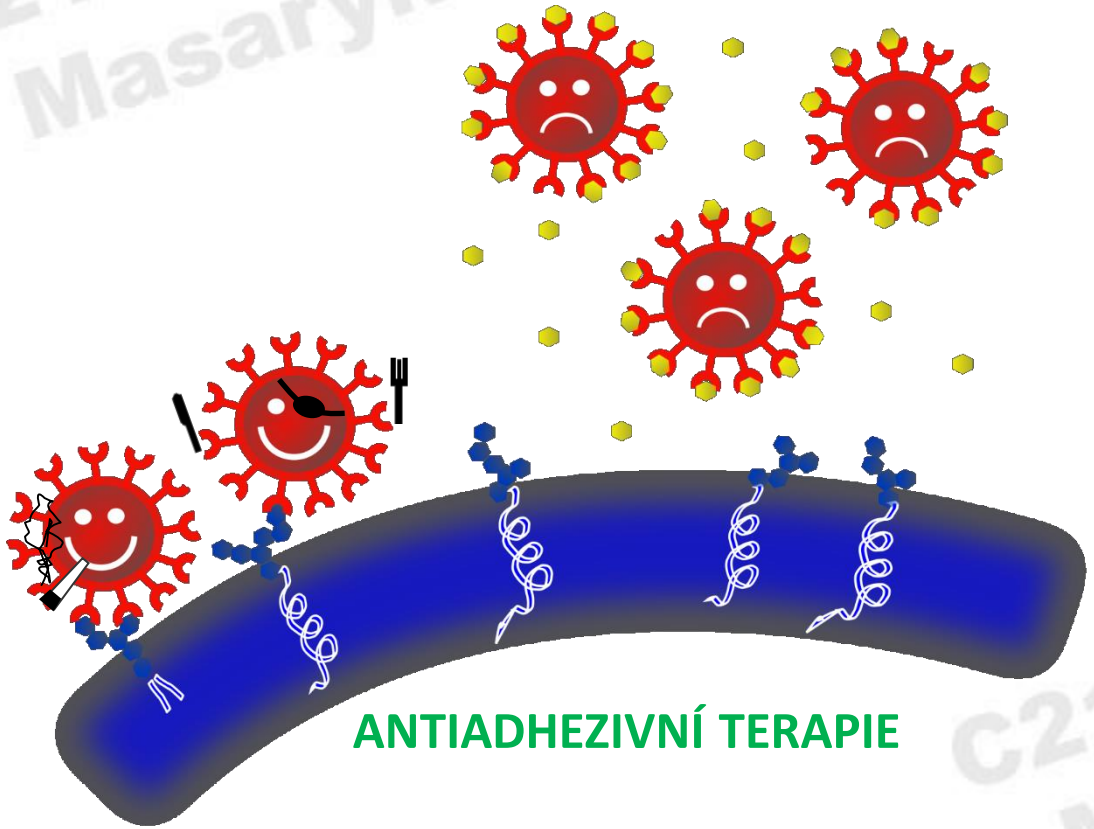
Multivalent glycoconjugates as anti-pathogenic agents†

Cite this: *Chem. Soc. Rev.*, 2013, **42**, 4709

Anna Bernardi,[a] Jesus Jiménez-Barbero,[b] Alessandro Casnati,[c] Cristina De Castro,[d] Tamis Darbre,[e] Franck Fieschi,[f] Jukka Finne,[g] Horst Funken,[h] Karl-Erich Jaeger,[h] Martina Lahmann,[i] Thisbe K. Lindhorst,[j] Marco Marradi,[k] Paul Messner,[l] Antonio Molinaro,[d] Paul V. Murphy,[m] Cristina Nativi,[n] Stefan Oscarson,[o] Soledad Penadés,[k] Francesco Peri,[p] Roland J. Pieters,[q] Olivier Renaudet,[r] Jean-Louis Reymond,[e] Barbara Richichi,[n] Javier Rojo,[s] Francesco Sansone,[c] Christina Schäffer,[l] W. Bruce Turnbull,[t] Trinidad Velasco-Torrijos,[u] Sébastien Vidal,[v] Stéphane Vincent,[w] Tom Wennekes,[x] Han Zuilhof[xy] and Anne Imberty*[z]



ANTIADHEZIVNÍ TERAPIE

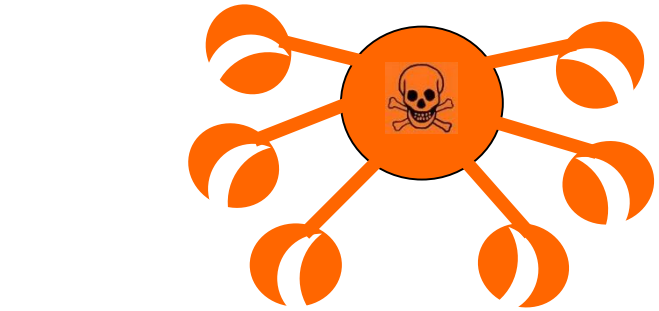
Published OnlineFirst January 29, 2016; DOI: 10.1158/1535-7163.MCT-15-0633

Large Molecule Therapeutics

Molecular Cancer Therapeutics

Gastric Adenocarcinomas Express the Glycosphingolipid Gb_3/CD77: Targeting of Gastric Cancer Cells with Shiga Toxin B-Subunit

Philipp Emanuel Geyer[1], Matthias Maak[1], Ulrich Nitsche[1], Markus Perl[1], Alexander Novotny[1], Julia Slotta-Huspenina[2], Estelle Dransart[3,4,5], Anne Holtorf[1], Ludger Johannes[3,4,5], and Klaus-Peter Janssen[1]

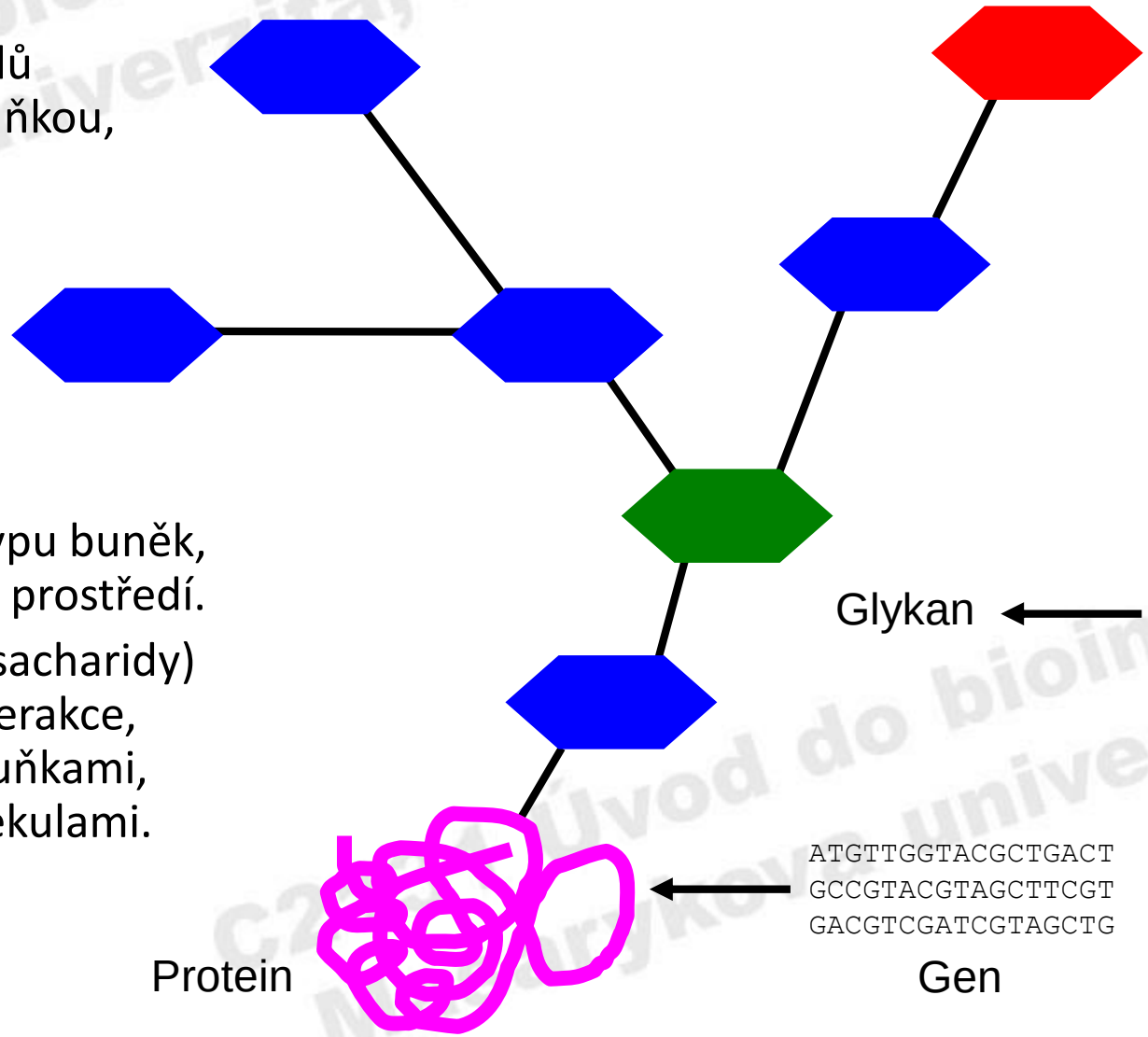


„DRUG-TARGETING“

Jak jsou glykoproteiny kódovány v genomu?

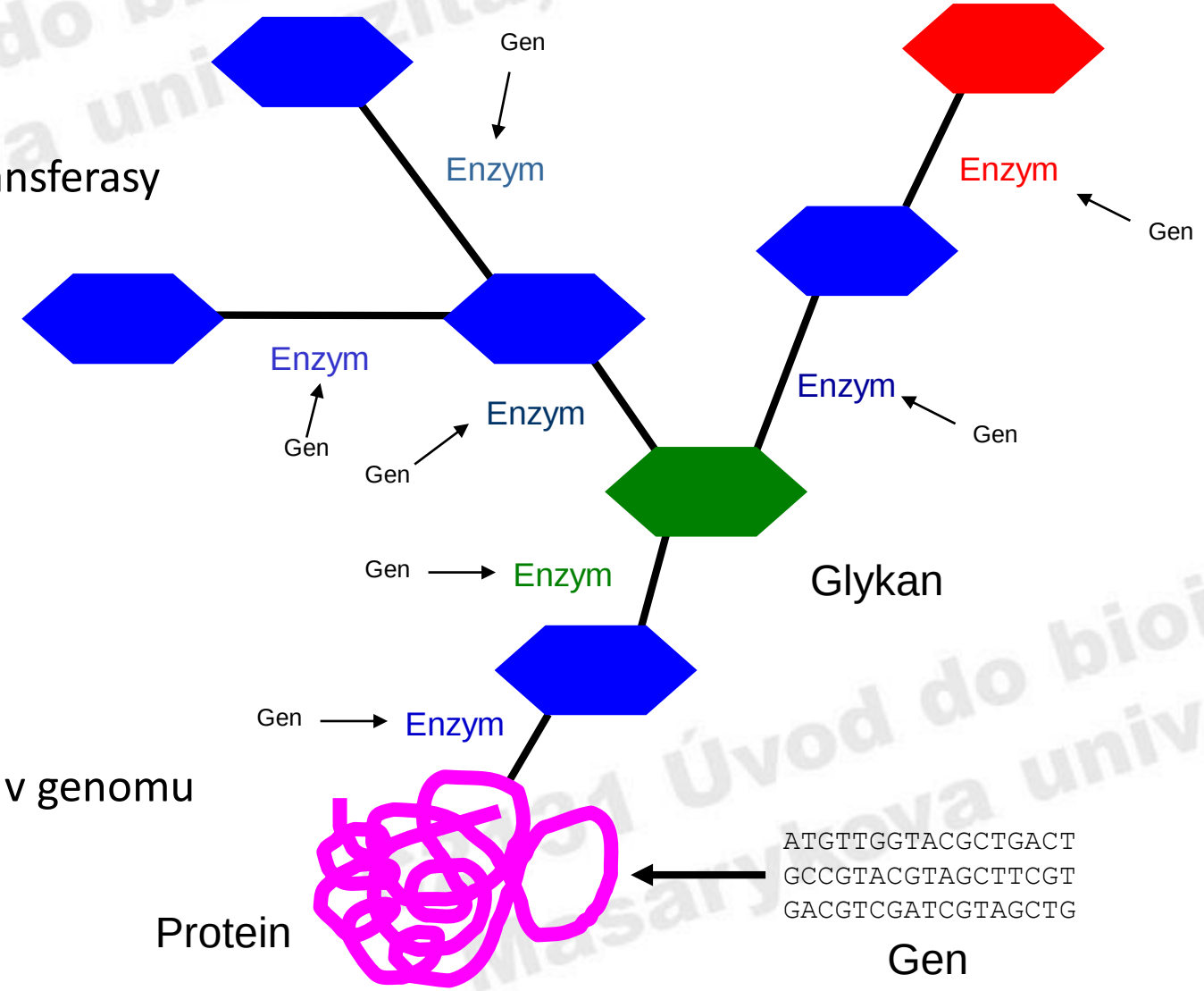
- **Glykom** – soubor všech sacharidů produkovaných organismem (buňkou, tkání) v daném čase za daných podmínek.

- **Glykosylace buněk** – závisí na typu buněk, (zdravotním) stavu buněk, věku, prostředí.
- **Glykosylace buněk** (povrchové sacharidy) – využívá se pro komunikaci, interakce, **specifické rozpoznávání** mezi buňkami, popřípadě mezi buňkami a molekulami.



Jak jsou glykoproteiny kódovány v genomu?

Enzymy = glykosyltransferasy

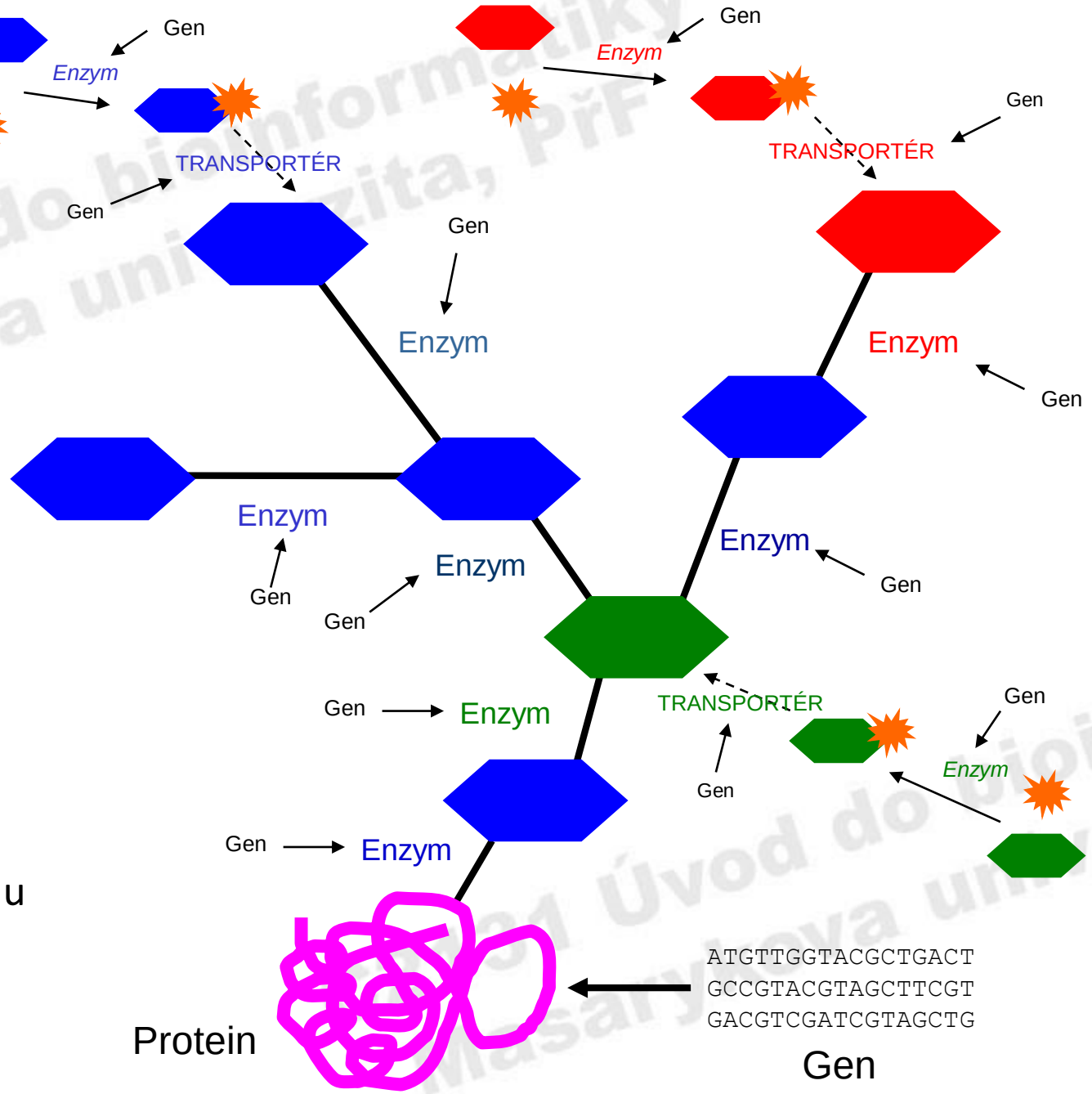


Struktura glykanů je v genomu kódována nepřímo

Enzymy = glykosyltransferasy, syntéza aktivovaných cukrů

Nutná účast transportních proteinů!

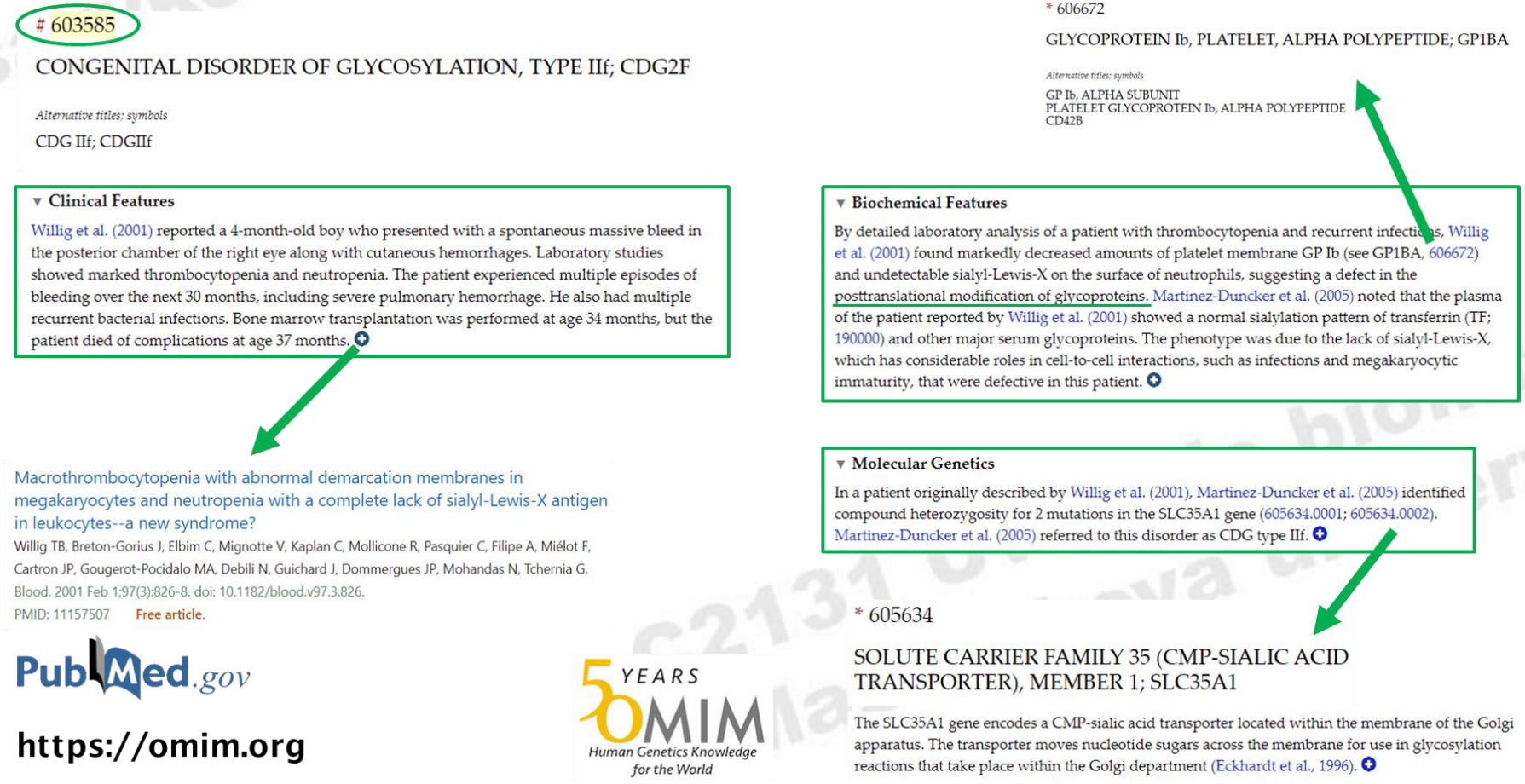
Struktura glykanů je v genomu kódována nepřímo



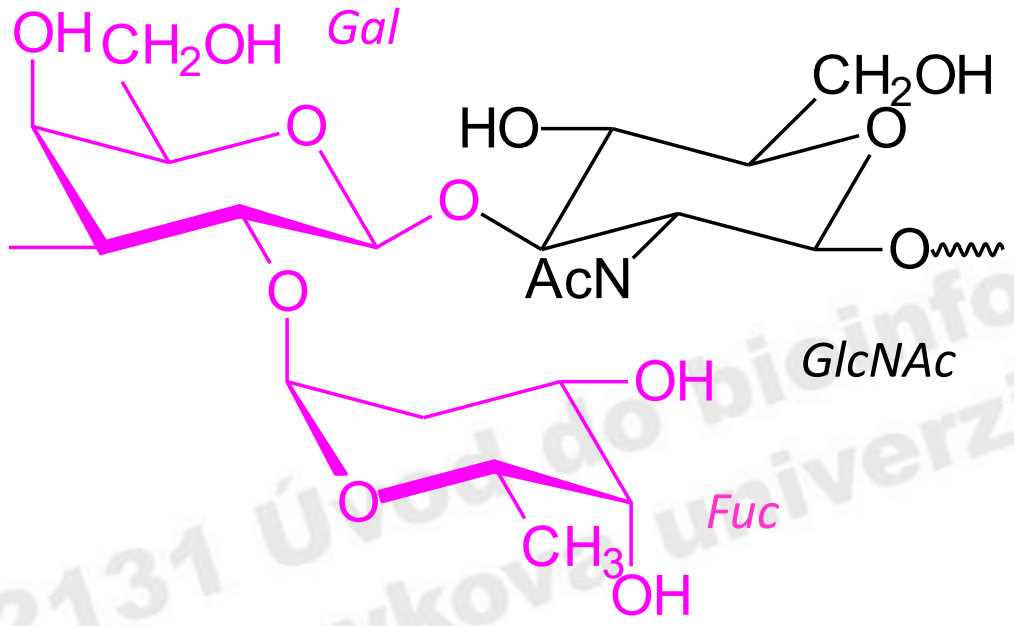
Glykosylace

- **CDG (congenital disorders of glycosylation) – dědičné poruchy glykosylace.**

  Glykosylace proteinů je složitý proces (syntéza aktivovaných cukrů, glykosyltransferasy, modifikace glykanů, glykosidasy), různých poruch glykosylace jsou tedy ***desítky***.

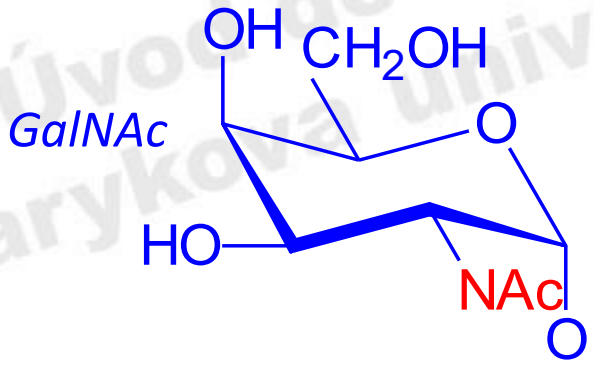


Dědičnost krevních skupin



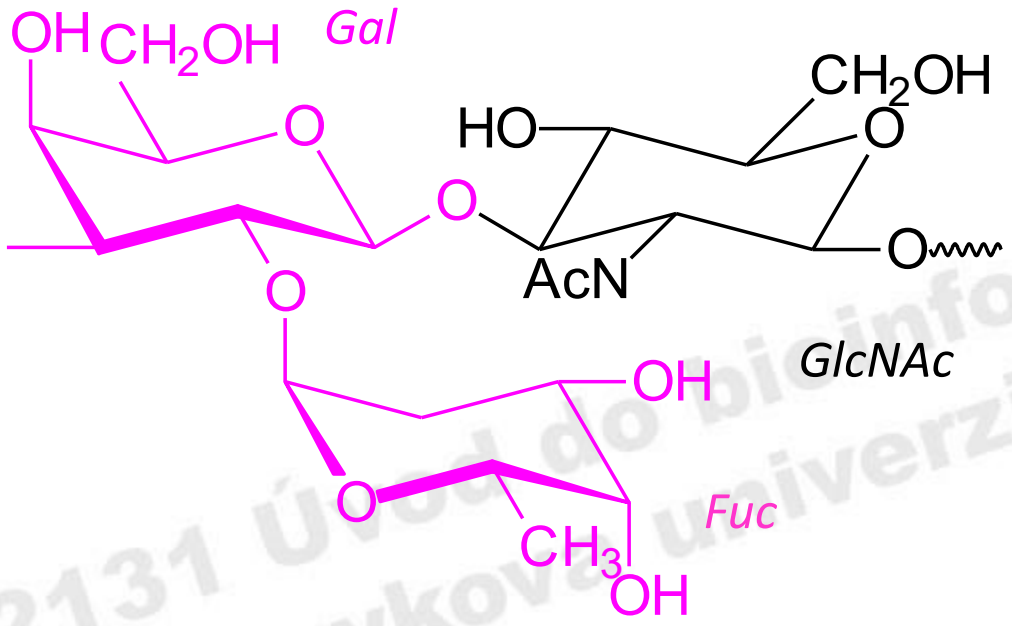
Tři varianty (alely) jednoho genu pro glykosyltransferasu (lokus AB0 na 9. chromozomu)

Dědičnost krevních skupin



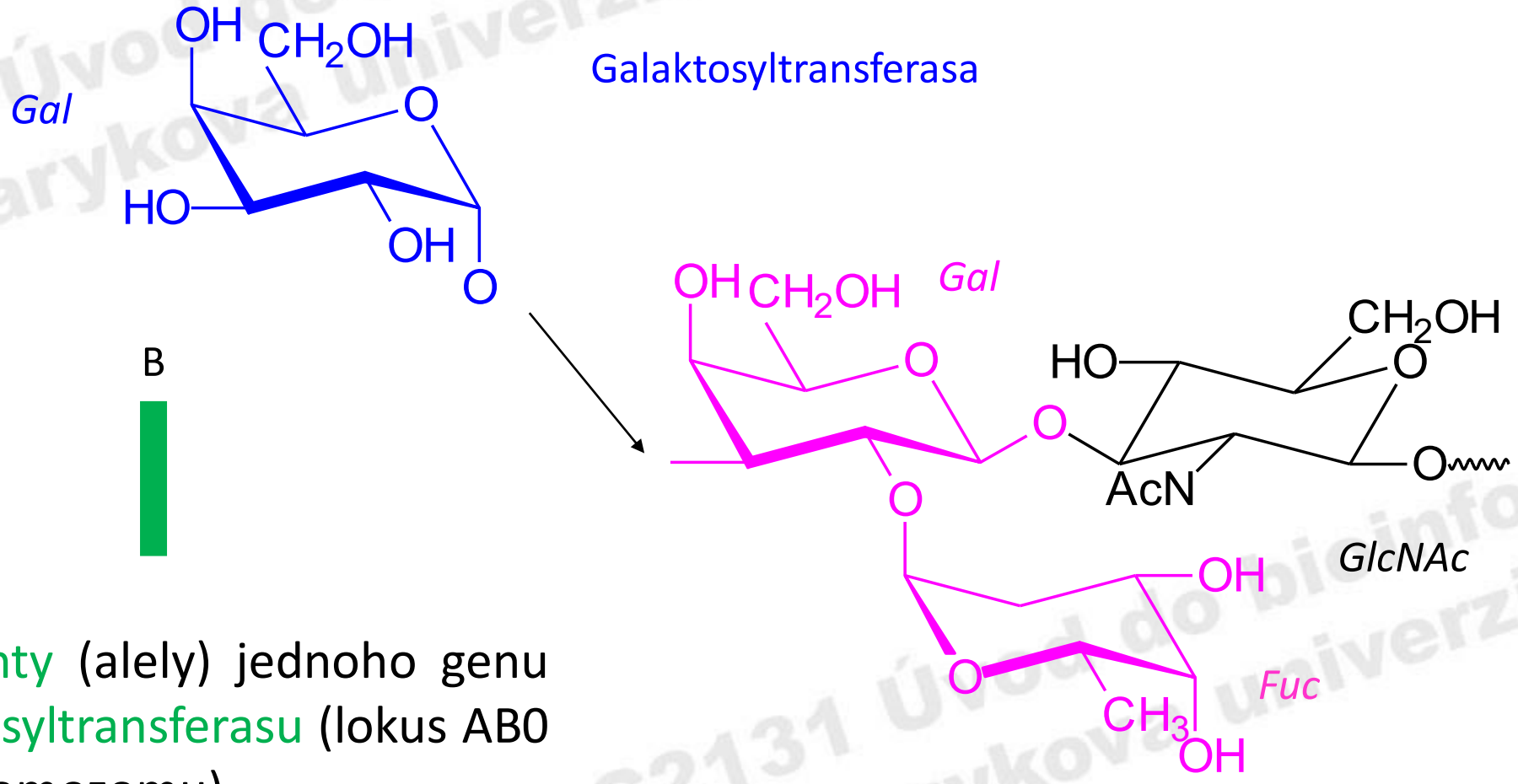
A

N-acetylgalaktosaminyltransferasa



Tři varianty (alely) jednoho genu pro glykosyltransferasu (lokus AB0 na 9. chromozomu)

Dědičnost krevních skupin

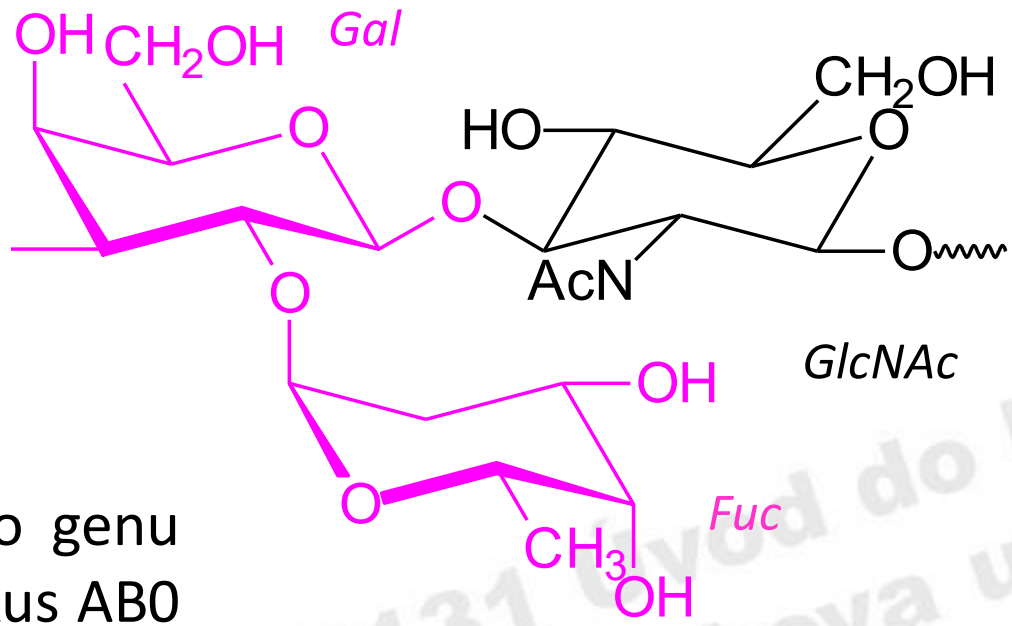


Tři varianty (alely) jednoho genu pro glykosyltransferasu (lokus AB0 na 9. chromozomu)

Dědičnost krevních skupin

Zkrácená (nefunkční) varianta genu, způsobeno delecí jednoho nukleotidu a následným posunutím čtecího rámce

0



Tři varianty (alely) jednoho genu pro glykosyltransferasu (lokus AB0 na 9. chromozomu)

Glycoconj J (2013) 30:41–50
DOI 10.1007/s10719-012-9397-y

Genomics and epigenomics of the human glycome

Vlatka Zoldoš · Mislav Novokmet · Ivona Bečeheli · Gordan Lauc

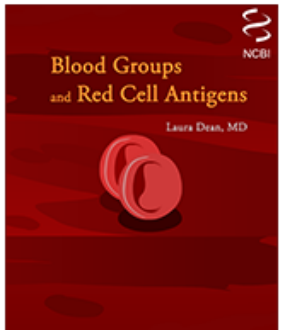
Received: 2 March 2012 / Revised: 11 May 2012 / Accepted: 14 May 2012 / Published online: 31 May 2012

Abstract The majority of all proteins are glycosylated and glycans have numerous important structural, functional and regulatory roles in various physiological processes. While structure of the polypeptide part of a glycoprotein is defined by the sequence of nucleotides in the corresponding gene, structure of a glycan part results from dynamic interactions between hundreds of genes, their protein products and environmental factors. The composition of the glycome attached to an individual protein, or to a complex mixture of proteins, like human plasma, is stable within an individual, but very variable between individuals. This variability stems from numerous common genetic polymorphisms reflecting in changes in the complex biosynthetic pathway of glycans, but also from the interaction with the environment. Environment can affect glycan biosynthesis at the level of substrate availability, regulation of enzyme activity and/or hormonal signals, but also through gene-environment interactions. Epigenetics provides a molecular basis how the environment can modify phenotype of an individual. The epigenetic information (DNA methylation pattern and histone code) is especially vulnerable to environmental effects in the early intrauterine and neo-natal development and many common late-onset diseases take root already at that time. The evidences showing the link between epigenetics and glycosylation are accumulating. Recent progress in high-throughput glycomics, genomics and epigenomics enabled first epidemiological and genome-wide association studies of the glycome, which are presented in this mini-review.

Keywords Glycosylation · Glycome · Genome-wide association study · Epigenetics · Gene-environment interactions

Genetics of protein glycosylation is very complex

According to the central dogma of molecular biology, function of each protein is determined by its structure, which is defined by the nucleotide sequence in the corresponding gene. However, in the case of glycan moieties of glycoproteins, there are several additional layers of complexity between genes and the final glycan structure. The final structure of each glycan is therefore not encoded directly in the genome

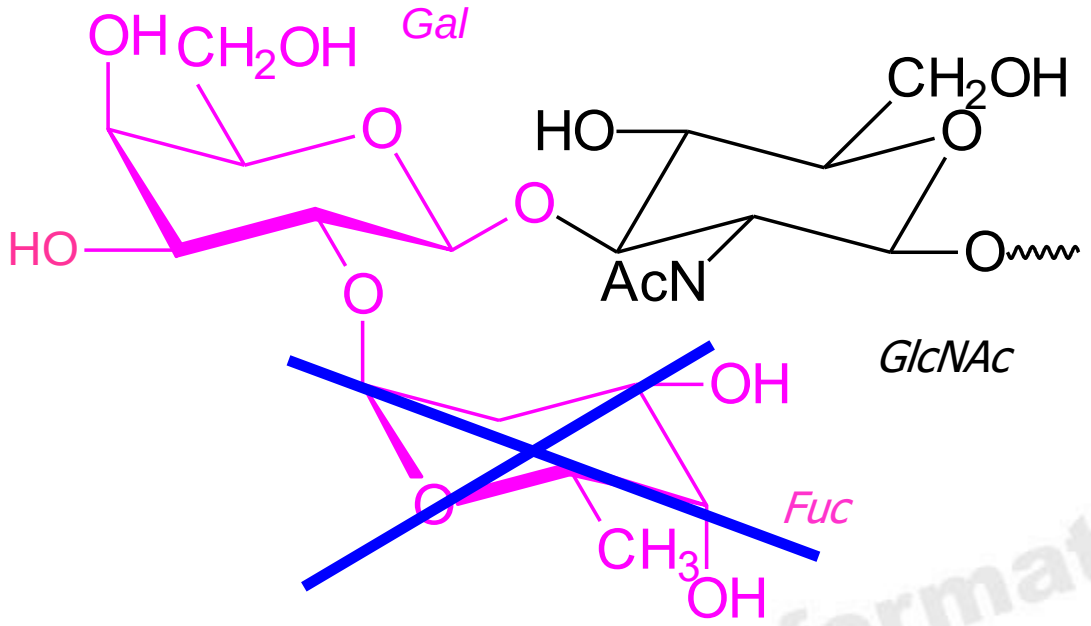


Dědičnost krevních skupin

ABO genotype in the offspring		ABO alleles inherited from the mother		
		A	B	O
ABO alleles inherited from the father	A	A	AB	A
	B	AB	B	B
	O	A	B	O

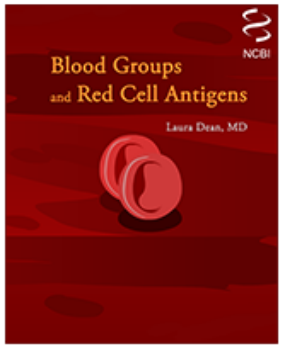
H antigen deficiency is known as the "Bombay phenotype" (h/h, also known as Oh) and is found in 1 of 10,000 individuals in India and 1 in a million people in Europe. There is no ill effect with being H deficient, but if a blood transfusion is ever needed, people with this blood type can receive blood only from other donors who are also H deficient. (A transfusion of "normal" group O blood can trigger a severe transfusion reaction.)

http://www.ncbi.nlm.nih.gov/books/NBK2261/



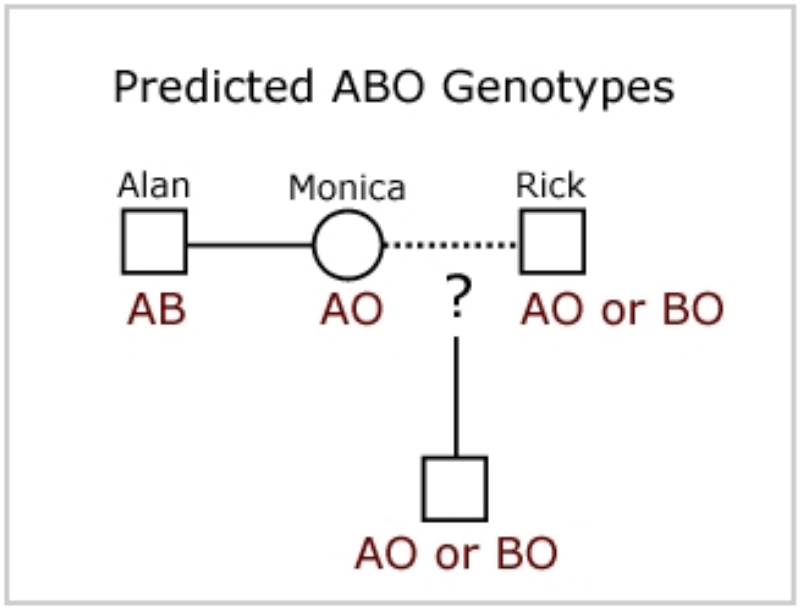
Bombajský fenotyp. Jedinci nejsou schopni vytvářet ani základní H antigen (defektní fukosyltransferasa). Vytvářejí se protilátky anti A, anti B i anti 0.

Působí problémy při transfuzích a testech paternity. Vhodné jako zápletka do seriálů.



Dědičnost krevních skupin

In the show "General Hospital", the father of Monica's child was in doubt. Monica had blood type A (genotype AO) and her child had blood type O (genotype OO). Because the child must inherit an O allele from the father, the father could have the genotype AO, BO, or OO. In other words, the child's father could have blood group A or B or O, which rules out Monica's husband Alan (type AB) and implicates Rick (type O).



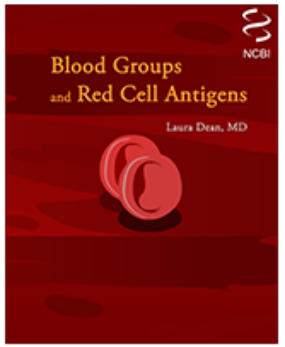
Monika má krevní skupinu A.

Alan má krevní skupinu AB.

Dítě má 0.

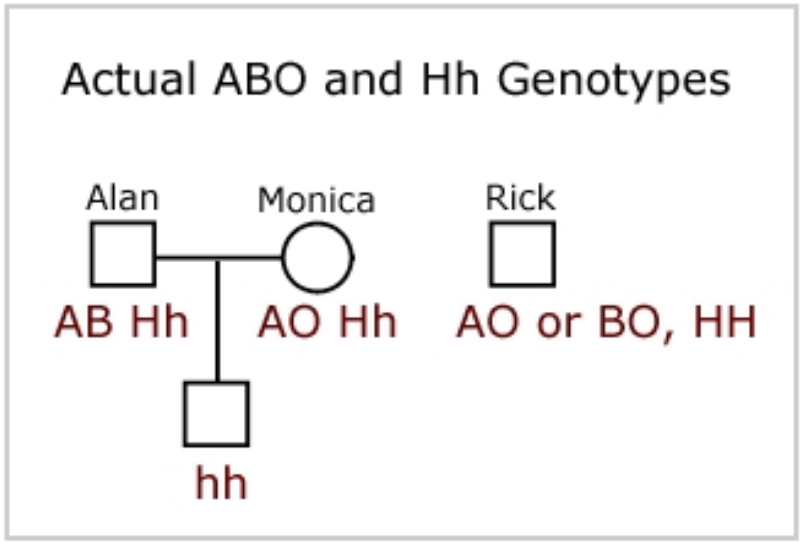
Podvedla Monika Alana s Rickem???

http://www.ncbi.nlm.nih.gov/books/NBK2261/



Dědičnost krevních skupin

However, Alan is the father! This is possible because both he and Monica are carriers of incomplete H deficiency (H/h). Their h/h child is unable to produce any ABO blood group antigens and so despite inheriting the A or B allele from Alan, the child's RBC's lack the A and B antigens as in blood type O.



Alan je tatínek! Ale možná je příbuzný s Monikou (vzhledem k vzácnosti alely h)...To by byl vhodný námět pro další díl…

„Because both parents must carry this recessive allele to transmit this blood type to their children, the condition mainly occurs in small closed-off communities where there is a good chance of both parents of a child either being of Bombay type, or being heterozygous for the h allele and so carrying the Bombay characteristic as recessive. Other examples may include noble families, which are inbred due to custom rather than local genetic variety.“

http://www.ncbi.nlm.nih.gov/books/NBK2261/

Cukry – zkratky a symboly

- Základní jednotky složitějších sacharidů jsou **monosacharidy**.
- NA/proteiny – základní jednotky (nukleotidy, aminokyseliny) jsou jasně definovány a jejich počet není velký.
- Monosacharidů je **mnoho**, proto u glykanů nelze (jednoduše) použít jednopísmenný kód. Problém: **vazby, větvení, modifikace**
- Vyvinuto a používáno mnoho způsobů, jak sacharidy znázornit.
- Na rozdíl od NA/proteinů se u cukrů velmi často využívá **grafické znázornění**.

Cukry – zkratky a symboly

UNION OF PURE AND APPLIED CHEMISTRY

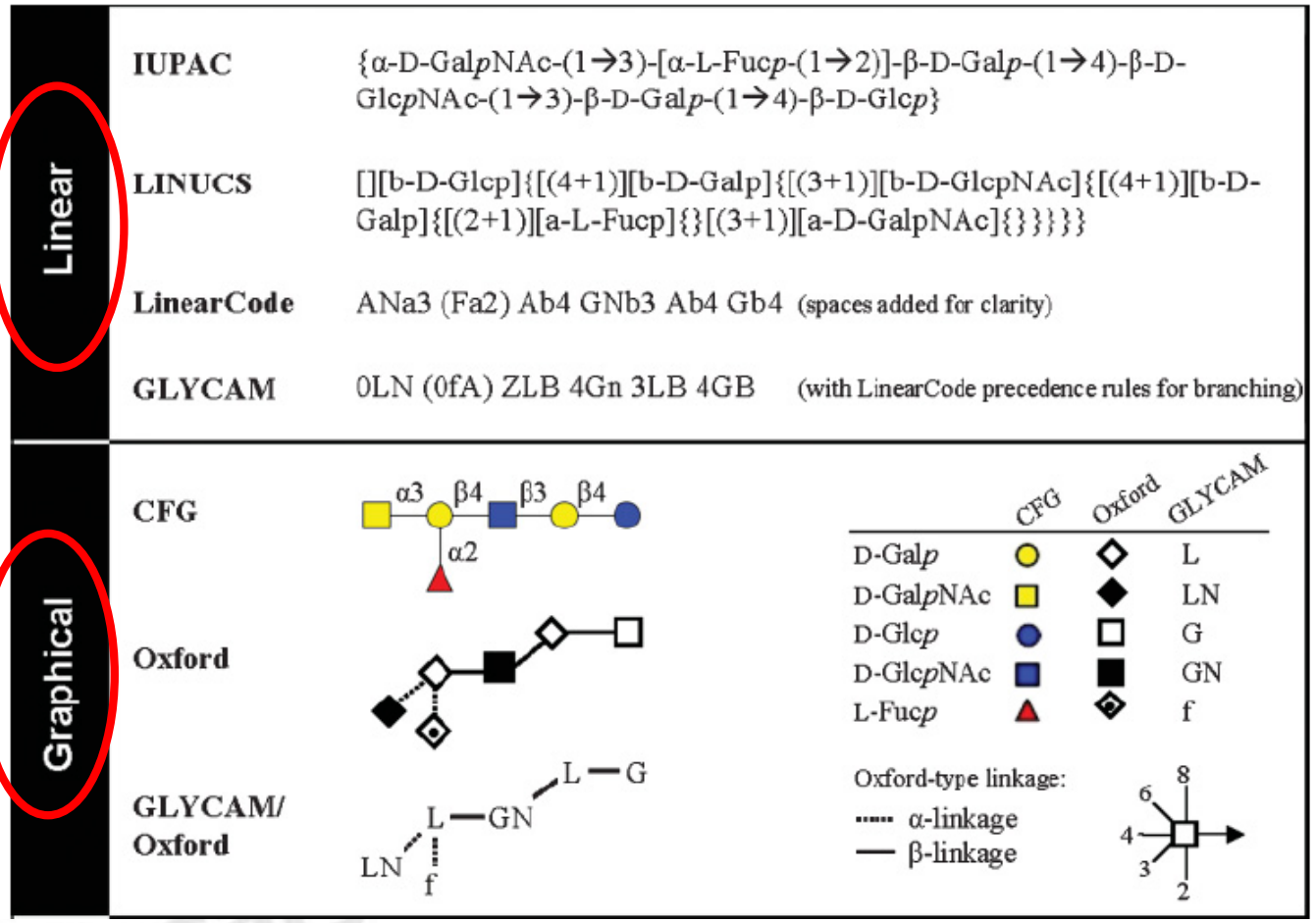
https://www.qmul.ac.uk/sbcs/iupac/2carb/

β-D-Galp-(1→4)-β-D-GlcpNAc-(1→2)-α-D-Manp-(1→
3
↑
1
α-L-Fucp

Gal(β1–4)GlcNAc-(β1–2)Man(α1–
|
Fuc(α1-3)

Gal(β1-4)[Fuc(α1-3)]GlcNAc(β1-2)Man(α1-

- **Tři IUPAC způsoby jak pomocí zkratek znázornit oligosacharid.**



Cukry – zkratky a symboly

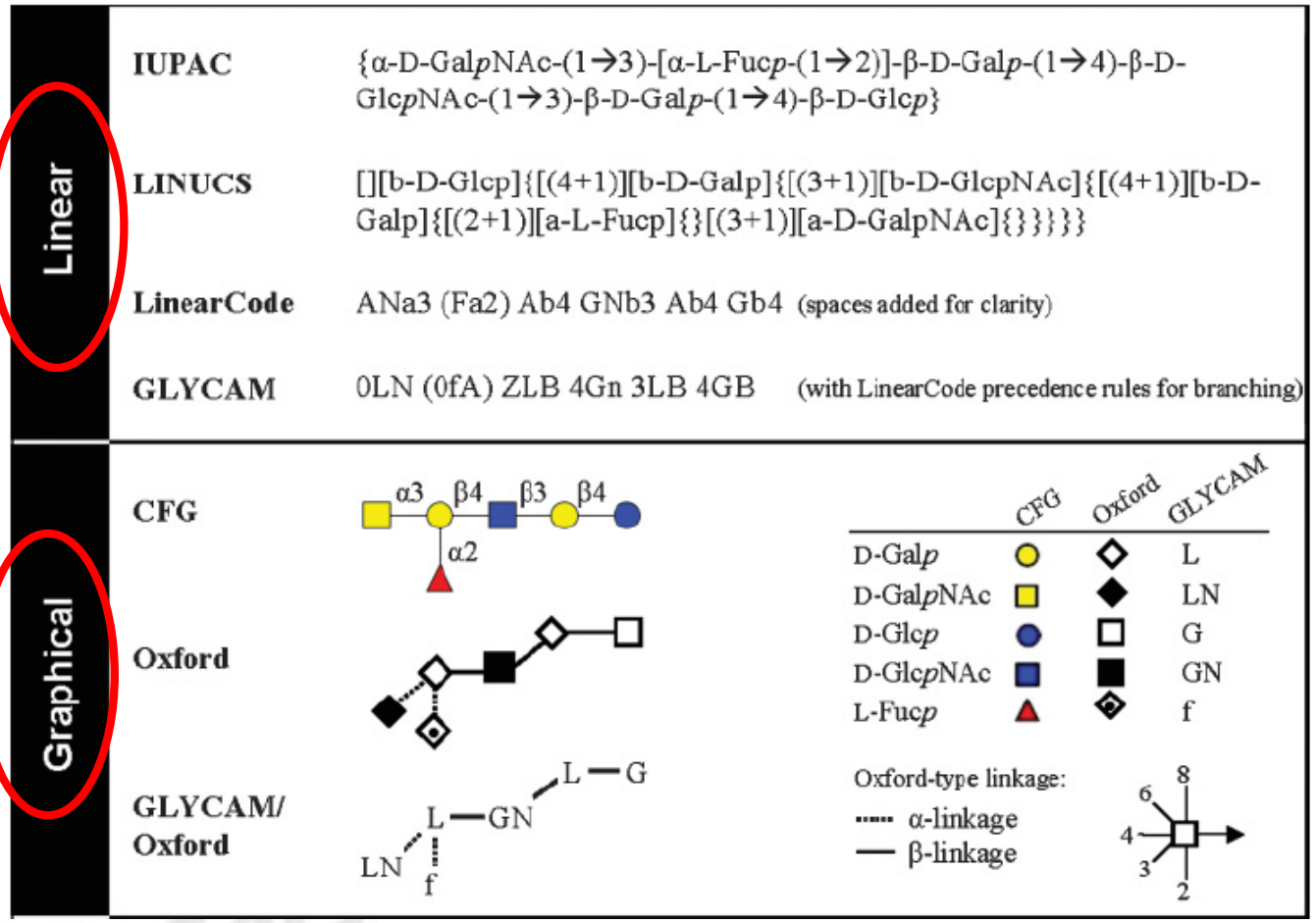
Standardizace symbolů:

Symbol Nomenclature for Glycans (SNFG)

https://www.ncbi.nlm.nih.gov/glycans/snfg.html

SHAPE	White (Generic)	Blue	Green	Yellow	Orange	Pink	Purple	Light Blue	Brown	Red
Filled Circle	Hexose	Glc	Man	Gal	Gul	Alt	All	Tal	Ido	
Filled Square	HexNAc	GlcNAc	ManNAc	GalNAc	GulNAc	AltNAc	AllNAc	TalNAc	IdoNAc	
Crossed Square	Hexosamine	GlcN	ManN	GalN	GulN	AltN	AllN	TalN	IdoN	
Divided Diamond	Hexuronate	GlcA	ManA	GalA	GulA	AltA	AllA	TalA	IdoA	
Filled Triangle	Deoxyhexose	Qui	Rha		6dGul	6dAlt		6dTal		Fuc
Divided Triangle	DeoxyhexNAc	QuiNAc	RhaNAc			6dAltNAc		6dTalNAc		FucNAc
Flat Rectangle	Di-deoxyhexose	Oli	Tyv		Abe	Par	Dig	Col		
Filled Star	Pentose		Ara	Lyx	Xyl	Rib				
Filled Diamond	Deoxynonulosonate		Kdn				Neu5Ac	Neu5Gc	Neu	Sia
Flat Diamond	Di-deoxynonulosonate		Pse	Leg		Aci		4eLeg		
Flat Hexagon	Unknown									
Pentagon	Assigned									

Symboly pro jednotlivé monosacharidy. Vzhledem k počtu monosacharidů je nutné využívat různé barvy i tvary.



Cukry – zkratky a symboly

Standardizace symbolů:

Symbol Nomenclature for Glycans (SNFG)

https://www.ncbi.nlm.nih.gov/glycans/snfg.html

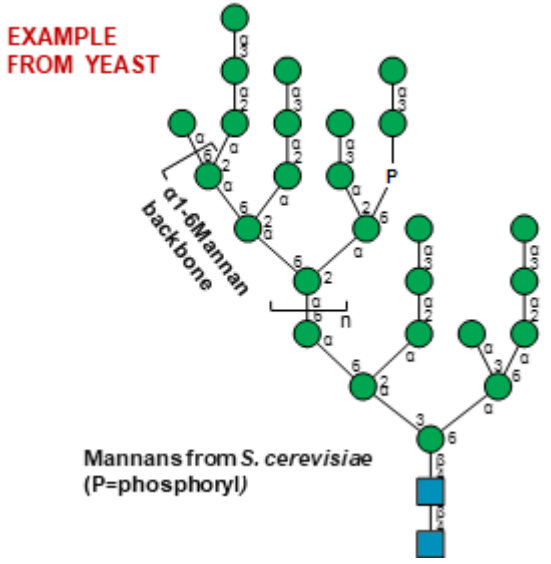
Významná část glykobioinformatických nástrojů je zaměřená na grafické znázornění cukrů.

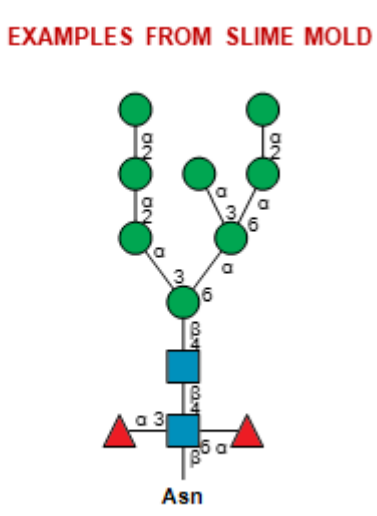
Symbol Nomenclature for Glycans (SNFG)

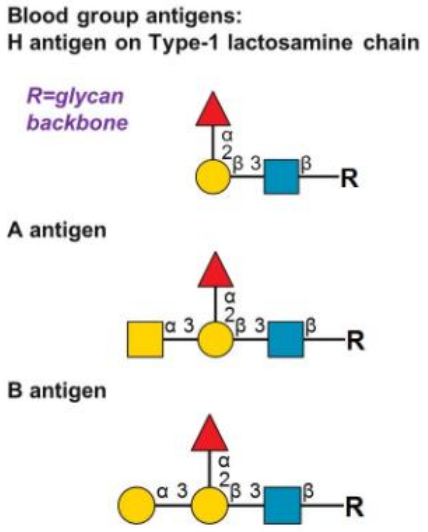
Standardization in drawing glycan structures is essential for efficient communication. The tools and methodology illustrated here have become widely accepted by the scientific community. Use of these symbols to represent monosaccharides is now strongly recommended for all manuscripts submitted to major journals and other publications.

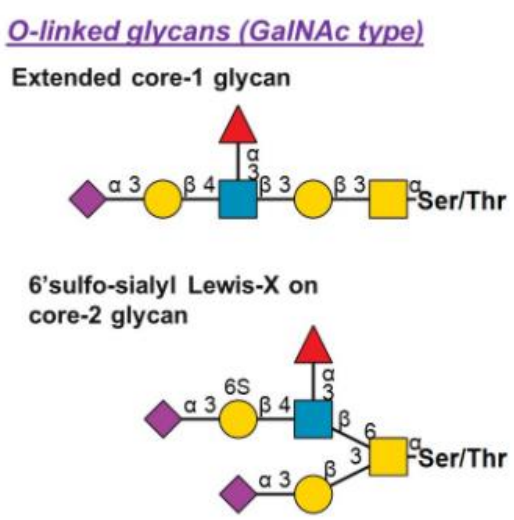
Citation:

- Symbol Nomenclature for Graphical Representation of Glycans, *Glycobiology* 25: 1323-1324, 2015. Citation link (PMID 26543186).
- Updates to the Symbol Nomenclature for Glycans guidelines, *Glycobiology* 29:620-624, 2019. Citation link (PMID 31184695).









Cukry – zobrazovací nástroje

DrawGlycan-SNFG

Render glycans and glycopeptides with fragmentation info. using the Symbolic Nomenclature for Glycans [SNFG]

http://www.virtualglycome.org/DrawGlycan/

IUPAC-condensed Input (glycan or glycopeptide):

Man(a2)Man(a6)[Man(a2)Man(a3)]Man(a6)Gal(a3)Fuc(a6)Man(a2)Man(a6)
[Man(a2)Man(a3)]Man(a6)Gal(a3)

Basic options:

Display Linkage: ON Linkage font size: 16 Text font size: 16

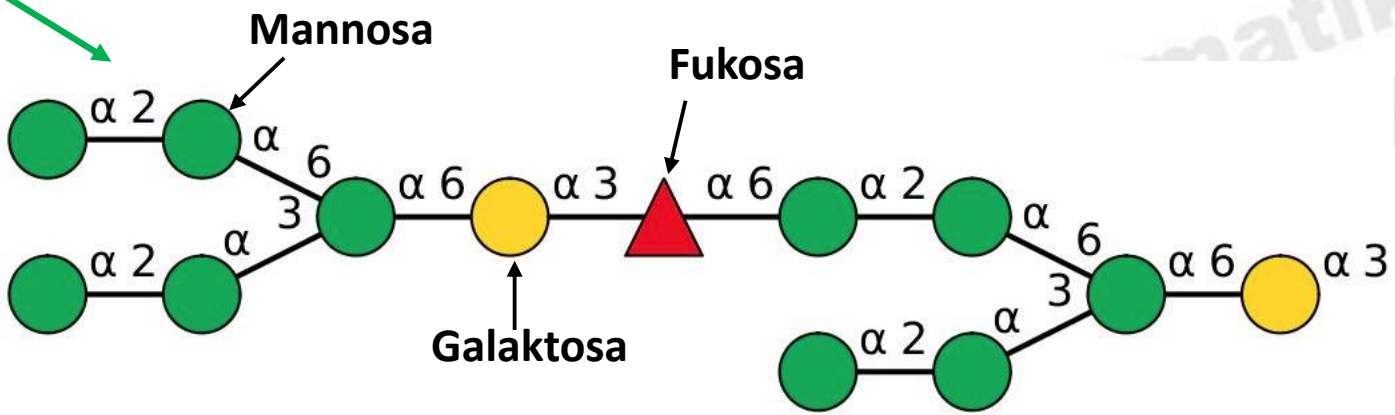
Symbol Size: Medium Orientation: Left

Other options (show/hide)

Mass Option: None Adduct: None

Draw

Molecular Weight: 2254.7562



Glykosylace

- **Glykosylace** je významná posttranslační modifikace.
- Ovlivňuje **strukturu** proteinů, jejich **aktivitu** i **funkci** (rozpustnost, stabilita, interakce, význam pro **imunitní systém**).
- Glykosylace probíhá u eukaryot i **prokaryot**.

A Repository of Experimentally Characterized Glycoproteins and Protein Glycosyltransferases of Prokaryotes

ProGlycProt Second Release

ProGlycProt is a manually curated, comprehensive repository of experimentally characterized glycoproteins and glycosyltransferases that are involved in protein glycosylation, in bacteria and archaea, exclusively. The website is a focused effort to provide concise and relevant information derived from rapidly expanding literature on prokaryotic glycoproteins, attached glycans, linkages, their glycosylating enzyme(s), their specificities, mutants, glycosylation linked genes, and genomic context thereof, in a cross-referenced, interactive manner... More>>>

ProGP ID	ProGP470 (Putative uncharacterized protein)
Validation Status	Characterized
Organism Information	
Organism Name	Burkholderia cenocepacia K56-2
Domain	Bacteria
Classification	Family: Burkholderiaceae Order: Burkholderiales Class: Betaproteobacteria Division or phylum: "Proteobacteria"
Taxonomic ID (NCBI)	985075
Protein Information	
Protein Name	Putative uncharacterized protein
UniProtKB/SwissProt ID	B4EB72
NCBI RefSeq	WP_006486887.1.
EMBL-CDS	CAR53291.1.
UniProtKB Sequence	>tr|B4EB72|B4EB72_BURCJ Putative exported protein OS=Burkholderia cenocepacia (strain ATCC BAA-245 / DSM 16553 / LMG 16656 / NCTC 13227 / J2315 / CF5610) GN=BCAL2973 PE=4 SV=1 MKSLVQAVVVAAALVAPVVSFAQSGSTITRAQVRAELVQLQQAGYNSARGEDPHYPEAIQ AATARIAEQQRSALAQAQGADVSGYGAQAQGASASGSRAMGVRPASAEEMKSLYRGS
Sequence length	117 AA
Subcellular Location	Outer membrane
Glycosylation Status	
Glycosylation Type	O- (Ser/Thr) linked
Experimentally Validated Glycosite(s) in Full Length Protein	S106
Glycosite(s) Annotated Protein Sequence	>tr|B4EB72|B4EB72_BURCJ Putative exported protein OS=Burkholderia cenocepacia (strain ATCC BAA-245 / DSM 16553 / LMG 16656 / NCTC 13227 / J2315 / CF5610) GN=BCAL2973 PE=4 SV=1 MKSLVQAVVVAAALVAPVVSFAQSGSTITRAQVRAELVQLQQAGYNSARGEDPHYPEAIQ AATARIAEQQRSALAQAQGADVSGYGAQAQGASASGSRAMGVRPAS*(106)AEEMKSLYRGS
Sequence Around Glycosites (21 AA)	GSRAMGVRPASAEEMKSLYRG
Technique(s) used for Glycosylation Detection	ZIC-HILIC,immunoblotting,tryptic digestion, and MS/MS analysis
Technique(s) used for Glycosylated Residue(s) Detection	MS/MS analysis
Glycan Information	
Glycan Annotation	Trisaccharide HexNAc-HexNAc-Hex.
BCSDB ID	12058
GlyTouCan	G71937MV

http://www.proglycprot.org/

ProGlycProt

Protein Glycosylation in Prokaryotes

Glykosylace

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554 Review TRENDS in Microbiology Vol.11 No.12 December 2003

Sweet new world: glycoproteins in bacterial pathogens

M. Alexander Schmidt[1], Lee W. Riley[2] and Inga Benz[1]

[1]Institut für Infektiologie, Zentrum für Molekularbiologie der Entzündung (ZMBE), Von-Esmarch-Str. 56, D-48149 Münster, Germany
[2]Division of Infectious Diseases and Immunity, School of Public Health, University of California, 140 Warren Hall, Berkeley, CA 94720, USA

In eukaryotes, the combinatorial potential of carbohydrates is used for the modulation of protein function. However, despite the wealth of cell wall and surface-associated carbohydrates and glycoconjugates, the accepted dogma has been that prokaryotes are not able to glycosylate proteins. This has now changed and protein glycosylation in prokaryotes is an accepted fact. Intriguingly, in Gram-negative bacteria most glycoproteins are associated with virulence factors of medically significant pathogens. Also, important steps in pathogenesis have been linked to the glycan substitution of surface proteins, indicating that the glycosylation of bacterial proteins might serve specific functions in infection and pathogenesis and interfere with inflammatory immune responses. Therefore, the carbohydrate modifications and glycosylation pathways of bacterial proteins will become new targets for therapeutic and prophylactic measures. Here we discuss recent findings on the structure, genetics and function of glycoproteins of medically important bacteria and potential applications of bacterial glycosylation systems for the generation of novel glycoconjugates.

http://www.proglycprot.org/

ProGlycProt

Protein Glycosylation in Prokaryotes

Predikce glykosylace

- **Glykosylace** je významná posttranslační modifikace.
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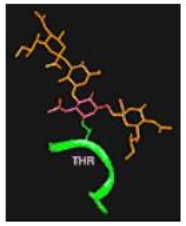
- Glykosylace probíhá u eukaryot i **prokaryot**.

NetOGlyc - 4.0
O-GalNAc (mucin type) glycosylation sites in mammalian proteins
The NetOglyc server produces neural network predictions of mucin type GalNAc O-glycosylation sites in mammalian proteins.

DictyOGlyc - 1.1
O-(alpha)-GlcNAc glycosylation sites (trained on Dictyostelium discoideum proteins)



The DictyOGlyc server produces neural network predictions for GlcNAc O-glycosylation sites in *Dictyostelium discoideum* proteins.

NetCGlyc - 1.0
C-mannosylation sites in mammalian proteins
The NetCGlyc 1.0 produces neural network predictions of C-mannosylation sites in mammalian proteins.

NetNGlyc - 1.0
N-linked glycosylation sites in human proteins

The NetNglyc server predicts N-Glycosylation sites in human proteins using artificial neural networks that examine the sequence context of Asn-Xaa-Ser/Thr sequons.

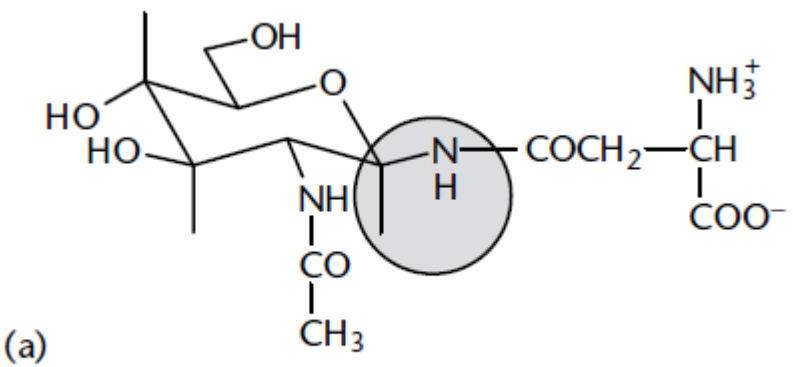
https://services.healthtech.dtu.dk/

MINI REVIEW

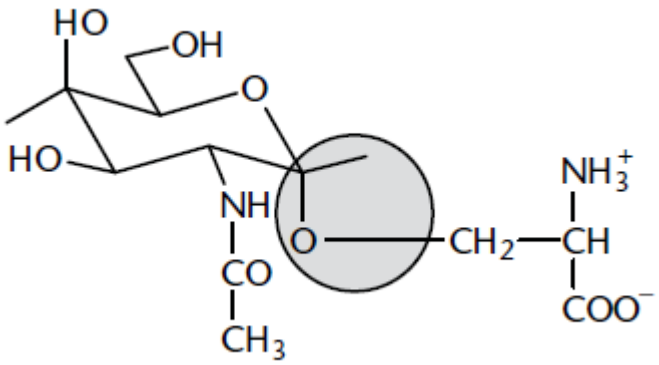
Protein glycosylation: nature, distribution, enzymatic formation, and disease implications of glycopeptide bonds

Predikce glykosylace

- Predikce glykosylace: *N*-glykosylace x *O*-glykosylace



(a)



(b)

N-glykosylace asparaginu

O-glykosylace hydroxylové skupiny serinu nebo threoninu

Glycoproteins

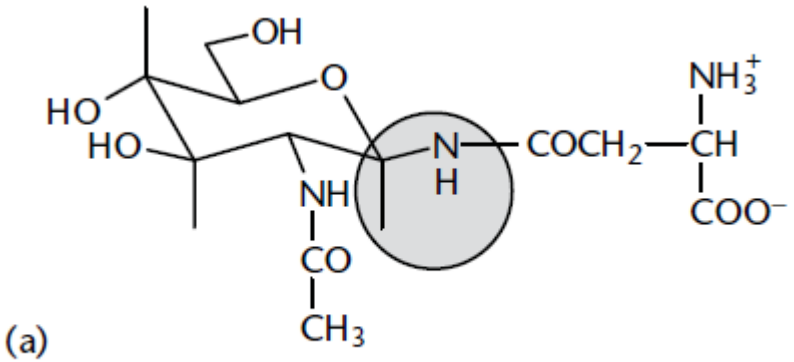
Tony Merry, *University of Manchester, Manchester, UK*
Sviatlana Astrautsova, *Grodno State Medical University, Grodno, Belarus*

Based in part on the previous version of this Encyclopedia of Life Sciences (ELS) article, ''Glycoproteins'' by ''Terry D Butters''.

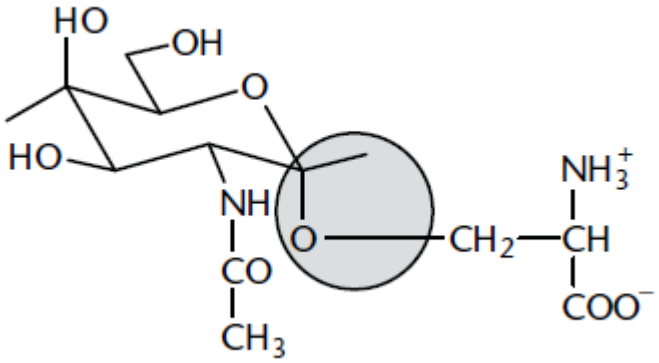
Glykosylace chrání proteiny před proteolýzou, ovlivňuje strukturu a interakce proteinů, uplatňuje se v interakcích imunitního systému.

Predikce glykosylace

- Predikce glykosylace: *N*-glykosylace x *O*-glykosylace



(a)



(b)

N-glykosylace asparaginu

Asn-X-Ser(Thr), X nesmí být Pro

Asn-X-C – nekanonický motiv

Záleží i na sousedních aminokyselinách, charakteru aminokyseliny „X“, konformaci místa.

O-glykosylace hydroxylové skupiny serinu nebo threoninu

Nemají jasně definovaný motiv

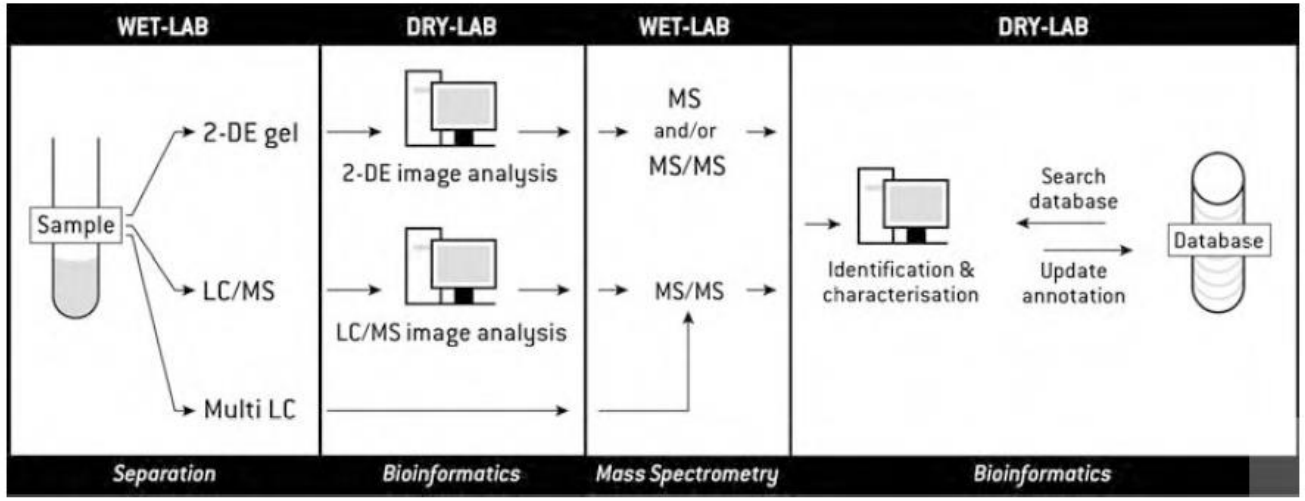
Identification of novel N-glycosylation sites at non-canonical protein consensus motifs

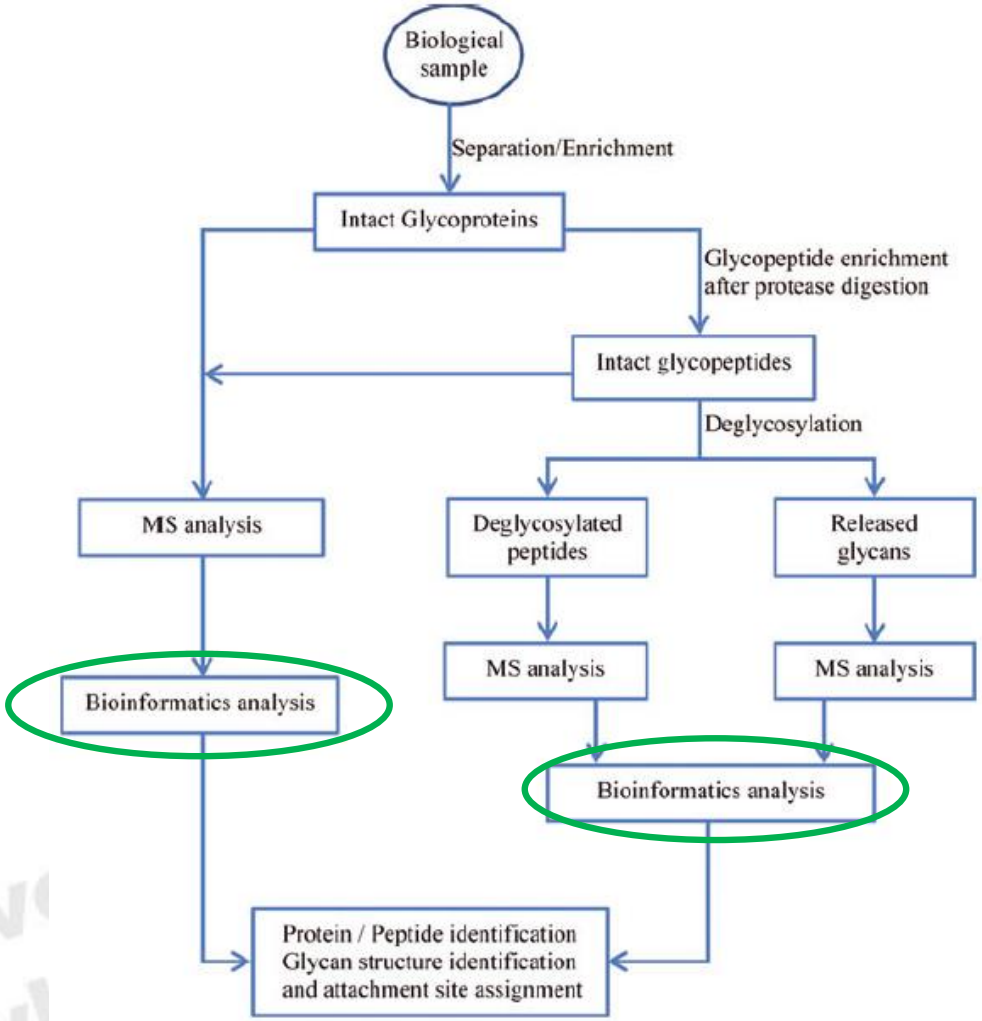
Mark S. Lowenthal*, Kiersta S. Davis, Trina Formolo, Lisa E. Kilpatrick, and Karen W. Phinney

Analýza glykanů

- Charakterizace glykanů: hmotnostní spektroskopie (**MS**), vysokoúčinná kapalinová chromatografie (**HPLC**), nukleární magnetická rezonance (**NMR**).

- Velká část softwarových nástrojů je zaměřena na zpracování a interpretaci experimentálních dat, **analýza glykanů je bez využití bioinformatiky velmi obtížná (prakticky nemožná)...**





Feng Li[1,2], Olga V. Glinskii[1,3] and Vladislav V. Glinsky[1,2]

Proteomics 2013, *13*, 341–354 DOI 10.1002/pmic.201200149

Cukry – 3D struktura

- Co nás zajímá – struktury **glykoproteinů**, struktury sacharidů v **komplexu** s proteiny (**lektiny, enzymy, protilátky**).
- **RTG** krystalografie. Problém: **velká flexibilita sacharidů** (ve struktuře je viditelná jen část glykanu).

  Problém: Kvalita 3D struktur sacharidů v PDB může být **nízká**...

- Určení struktury **komplexních** sacharidů je obecně problém.

  NMR – tradiční metoda pro určení struktury oligosacharidů (práce v roztoku), problémy s přiřazením signálů a vyhodnocením dat (malé rozdíly mezi jednotlivými jádry).
- **Molekulové modelování** sacharidů je často **nezbytnou** součástí interpretace experimentálních dat.

Cukry – 3D struktura

- Co nás zajímá – struktury **glykoproteinů**, struktury sacharidů v **komplexu** s proteiny (**lektiny, enzymy, protilátky**).
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  Molekulové modelování sacharidů je často **nezbytnou** součástí interpretace experimentálních dat.

It should be noted that under physiological conditions oligosaccharides are frequently highly flexible, and a single static structure is an incomplete model. For this reason, the user is encouraged to employ molecular dynamics simulations to develop a more complete understanding of the spatial and dynamic properties of their system.

All builders at GLYCAM-Web generate molecular structure files that can be used in visualization programs or as input for simulations. For the builders that generate 3D structures from a primary sequence (e.g., DManpb1-6DGlcpNAcb1-OH), we offer the interfaces listed below for setting the primary sequence.

GLYCAM

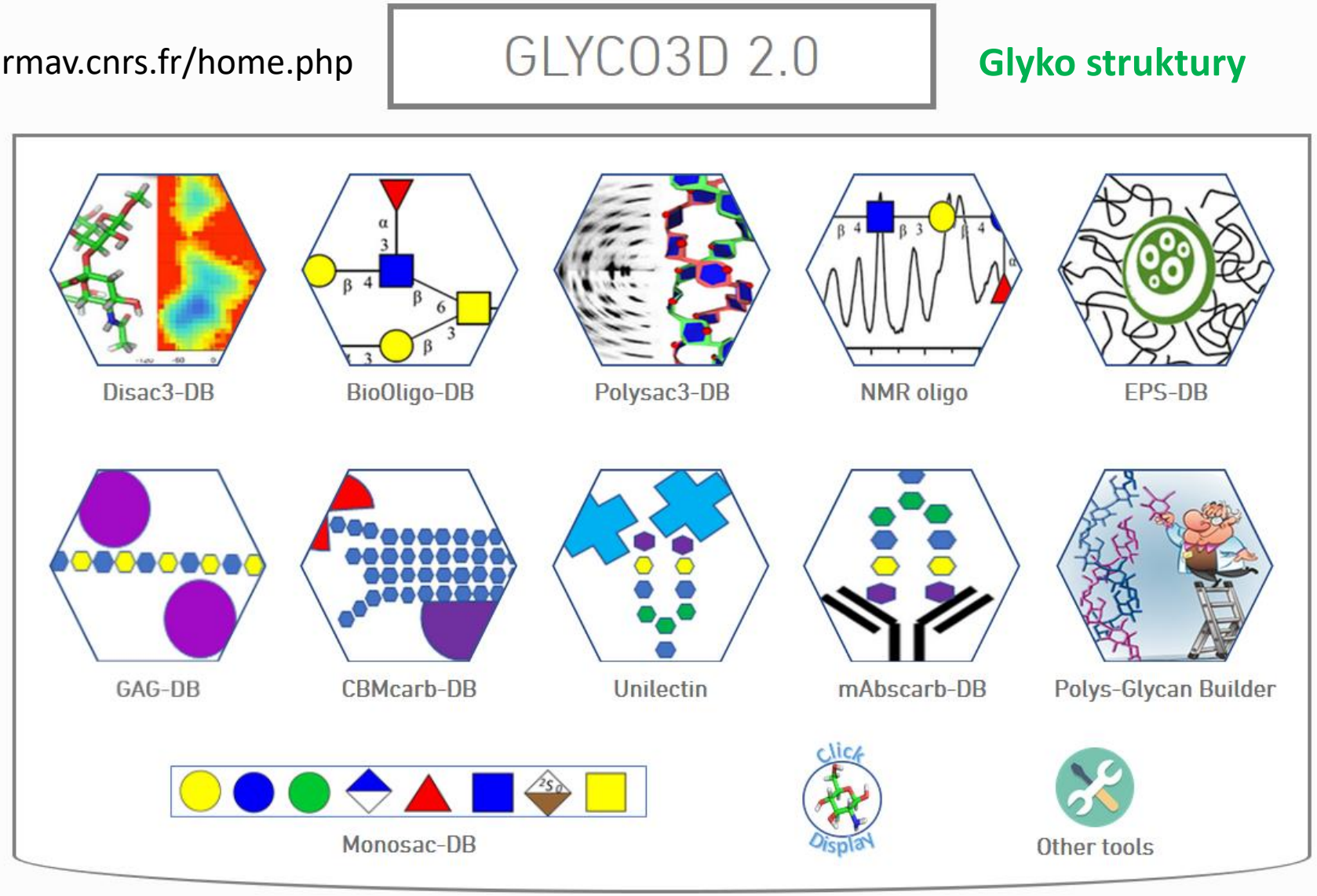
http://glycam.org/

Glykobioinformatika – databáze

- Databáze obsahující informace o **proteinech** (sacharidy jsou součást glykoproteinů, lektiny).
- Vlastní databáze **sacharidů** (struktury).
- Databáze **enzymů** a **drah** účastnících se syntéz a odbourávání glykanů (sacharidů).
- Informace o **interakcích** protein-sacharid
- **„Glykocentra“ – sdružené databáze, vlastní specializované databáze, analytické nástroje**

„Glykocentra“

http://glyco3d.cermav.cnrs.fr/home.php



Glyko struktury

„Glykocentra“

Cermav cnrs Glyco@Alps UGA Université Grenoble Alpes SIB Swiss Institute of Bioinformatics UNIVERSITÉ DE GENÈVE

Unified exploration platform for manually curated and predicted lectins

UniLectin3D
Curated and classified lectin 3D structures

PropLec
Predicted β-propeller lectins

LectomeXplore
Predicted lectins in all available species from all kingdoms

MycoLec
Predicted lectins in fungal genomes

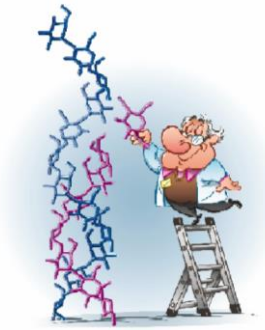
TrefLec
Predicted β-trefoil lectins

Glyco3D is a portal of databases covering the three-dimensional features of monosaccharides, disaccharides, oligosaccharides (Conformations and NMR spectra), polysaccharides, glycosyltransferases, lectins, monoclonal antibodies against carbohydrates, and glycosaminoglycan-binding proteins. These databases have been developed with non-proprietary software and they are opened freely to the scientific community. Each individual database stands by itself as it covers a particular field of structural glycosciences.

Glyco3D

http://glyco3d.cermav.cnrs.fr/home.php

POLYS GLYCAN BUILDER



- ALGEA BUILDER
- BACTERIA BUILDER
- GAG BUILDER
- N-O LINKED BUILDER
- PLANT BUILDER

POLYSAC3DB

Identifikace a izolace nových lektinů

GATAGCGTAATGATCGGCTGGCTGCCGCATTTCATGCTGGTTTCCCAACGAAAAT
TACAGGTGGTCGCGCCCGCCGCCAGCACATCGCTGCGCCAATAATGATCTTTCAG
GGTGGCGGCATCACGCACTTCCAGTTCGATCGGGGCAACAATGCCGGCATCTTTC
AGCGCGGTTTCGCGCAGATGCAGCTGATCACCCGGGCTCAGACCGGTAAACAGAC
CATACAGGTGGCGACCATCAATCACGGTCGGGGCGGCCGGATCACGGCTGGCTTC

Genomy

EDRPIKFSTEGATSQSYKQFIEALRERLRGGLIHD
IPVLPDPTTLQERNRYITVELSNSDTESIEVGIDV
TNAYVVAYRAGTQSYFLRDAPSSASDYLFTGTDQH
SLPFYGTYGDLERWAHQSRQQIPLGLQALTHGISF
FRSGGNDNEEKARTLIVIIQMVAEAARFRYISNRV

Známé lektiny

Bioinformatika

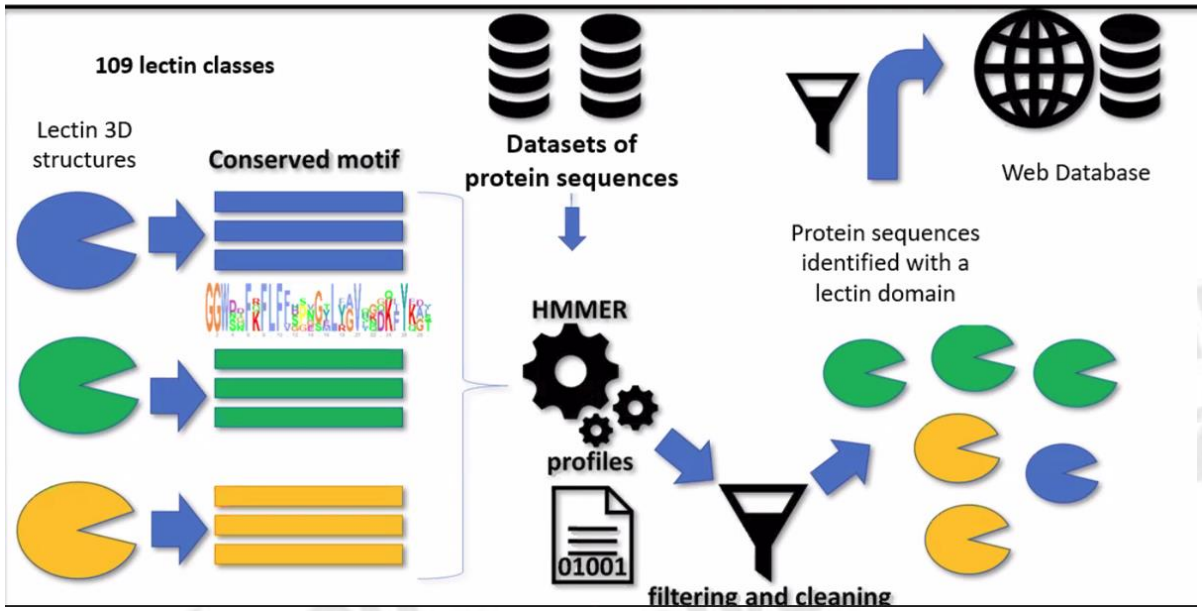
- ✓ Nové lektiny
- ✓ Levné
- ✓ Online databáze!

LectomeXplore - A database of predicted lectins

What is LectomeXplore ?

LectomeXplore is a module dedicated to the exploration of predicted lectins for each class from UniLectin3D classification. Translated genomes (proteomes) released in the UniProtKB and RefSeq sequence databases and in the PDB structure database were screened to identify the lectome (complete set of lectins) of the corresponding species.

Workflow of lectin domains prediction



LectomeXplore
Predicted lectins in all available species from all kingdoms

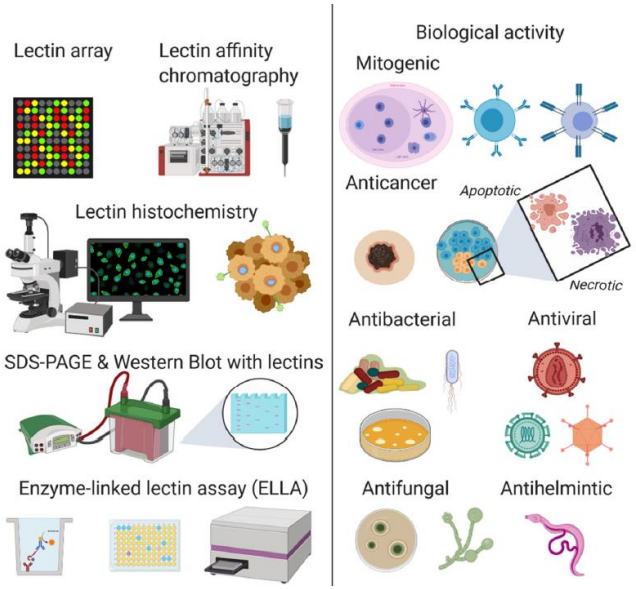
https://www.unilectin.eu/predict/

MycoLec
Predicted lectins in fungal genomes

https://www.unilectin.eu/mycolec/

Identifikace a izolace nových lektinů

- Práce s komplexním přírodním vzorkem.
- Malé množství vzorku (např. klíště), drahý vzorek, špatně dostupný.
- Nízká koncentrace lektinů.
- Poškození proteinů izolačním procesem.
- Pionýrský výzkum, rizikový.
- **Nové lektiny s dosud neznámou strukturou/vlastnostmi!**



Durian

Zdroj

Homogenizace

Frakcionace

Extrakce proteinů

Detekce lektinové aktivity

Purifikace lektinů

- [x] Nové lektiny
- [x] Nové **unikátní** lektiny

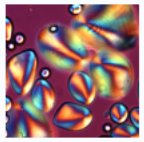
Glyko stránky

GlycoPedia

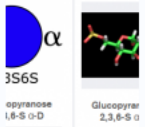
„Glyko drbna“

https://www.glycopedia.eu/

news | e-chapters | resources | search



Starch : Structure and Morphology
Serge Perez - Anne Imberty

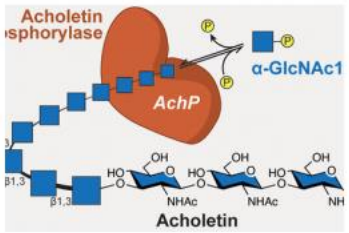


Library of Bio-active Monosaccharides. 1D,...
Serge Perez

18 mars 2022 news

Acholetin : A newly discovered Poly 1-3 β-D GlcNAc bacterial polysaccharide

Using genomic data and activity-based screening, the researchers identified a glycoside phosphorylase enzyme...

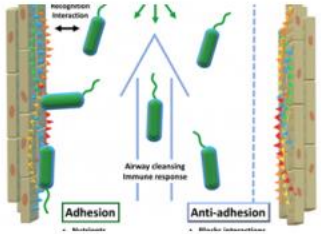


Acholetin

11 mars 2022 news

Glycomimetics against Multi-Drug Resistant Pathogens

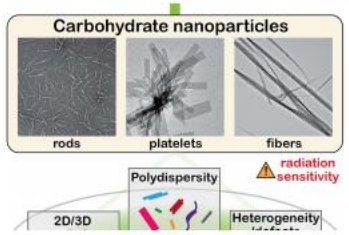
The collection of glycopedia virtual chapters has been extended with a new contribution Multi-drug resistant...



22 février 2022 news

Recent Advances in Electron Microscopy of Carbohydrate Nanoparticles

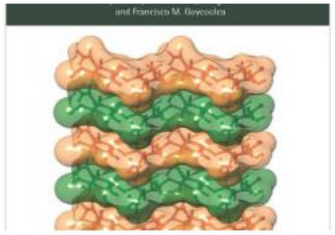
Carbohydrate nanoparticles, both naturally derived and synthetic ones, have attracted scientific and...



2 janvier 2022 news

Chitin and Chitosan in the Bioeconomy

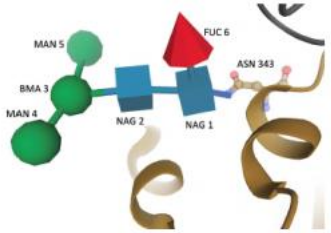
Chitin is the second most abundant natural polymer in the world after cellulose, mainly derived from the food...



20 décembre 2021 news

Modernized uniform representation of carbohydrate molecules in the Protein Data Bank

Carbohydrate molecules present in more than 14,000 Protein Data Bank (PDB) structures have recently been...



Lipidy

Lipidy jsou heterogenní skupina biomolekul nerozputných ve vodě a rozpustných v organických rozpouštědlech. Jsou to deriváty vyšších monokarboxylových kyselin a alifatických či alicyklických hydroxyderivátů nebo aminoderivátů. Patří do ní následující látky:

1. Tuky a oleje (acylglyceroly)
2. Glycerolipidy (glycerofosfolipidy, plasmalogeny, kardiolipin)
3. Sfingolipidy
4. Steroidy (cholesterol, žlučové kyseliny, steroidní hormony)
5. Izoprenoidy (ubichinon, plastochinon, dolichol)
6. Vitaminy rozpustné v tucích
7. Deriváty mastných kyselin (leukotrieny, prostaglandiny, prostacykliny, tromboxany)

Lipidy hrají v organismu roli jako zásobní látky, strukturální složky membrán, hormony a vitaminy.

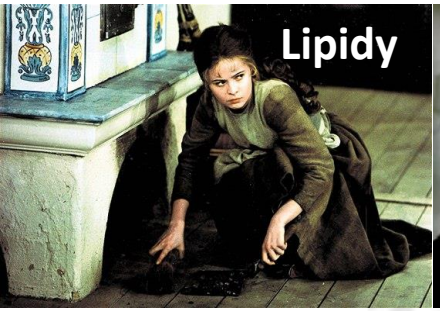
Základní pojmy z biochemie, V. Mikeš, Katedra biochemie PřF Masarykovy Univerzity v Brně, 2. doplněné vydání 2001

4.8.16 lipids

Small, biologically active molecules of variable structure, commonly defined by their solubility in non-polar solvents. Hydrophobic or amphipathic small molecules that may originate, entirely or in part, by the carbanion-based condensations of thioesters (fatty acyls, glycerolipids, glycerophospholipids, sphingolipids, saccharolipids, and polyketides) and/or by carbocation-based condensations of isoprene units (prenol lipids and sterol lipids).

Terminology of bioanalytical methods (IUPAC Recommendations 2018)

https://doi.org/10.1515/pac-2016-1120
Received November 21, 2016; accepted February 1, 2018



Lipidy a lipidomika

- **Zásobní látky (zdroj energie), mechanická ochrana, tepelná izolace, hormony, složky membrán, vitaminy**

Lipidomika

Lipidomika je vědní obor, který se zabývá studiem biochemických drah lipidů v biologických systémech. Slovo lipidom označuje veškeré lipidy v buňce, tkáni nebo organismu v daném čase a je podmnožinou metabolomu. Lipidomika je relativně mladý obor, který se rozvíjí v souvislosti s rychlými pokroky v lékařství, analytické chemii a informačních technologiích. Lipidy hrají velmi důležité role při vzniku a průběhu mnoha metabolických chorob jako je například obezita, ateroskleróza, cévní mozková příhoda, hypertenze nebo diabetes. V lipidomickém výzkumu se pracuje s velkými soubory dat, které kvantitativně popisují změny v obsahu a složení jednotlivých druhů lipidů. Analýza lipidomu znamená identifikaci a kvantifikaci tisíců molekulárních druhů lipidů, zkoumá se struktura a interakce s dalšími sloučeninami, jejich dynamika a změny, které nastanou v průběhu vzniku choroby. Informace získané z těchto studií hrají důležitou roli při objasňování vzniku a průběhu nemocí na molekulární úrovni.

Lipidy

Lipidy jsou strukturně různorodé chemické sloučeniny, které plní řadu klíčových biologických funkcí, například jako stavební složky buněčných membrán, zdroje a zásobárny energie, nebo jako signální molekuly. Lipidy mohou být obecně definovány jako hydrofobní nebo amphipatické molekuly, které alespoň částečně vznikají kondenzací thioesterů (mastné kyseliny, polyketidy, atd.) nebo isoprenových jednotek (prenoly, steroly, atd.). Lipidy se obecně dělí na "jednoduché" a "složené" lipidy, přičemž jednoduchými lipidy rozumíme ty, které při hydrolýze poskytují nanejvýš dva typy produktů, kdežto složené lipidy dávají při hodrolýze tři nebo více produktů.

LS **Lipidomická sekce**
České společnosti pro biochemii a molekulární biologii

http://lipidomics.uochb.cas.cz/lipidomika.html

Lipidomics: a global approach to lipid analysis in biological systems

Andrew D. Watson[1]

Department of Medicine, Division of Cardiology, David Geffen School of Medicine, University of California at Los Angeles, Los Angeles, CA 90095

1. **How to preserve and extract lipids?**
2. **What amount of lipids is present in the sample ?**
3. **How to fractionate a natural lipid extract?**
4. **What are the components present within each fraction?**
5. **What amounts of each component are present in the lipid extract?**

Analýza lipidů

http://cyberlipid.gerli.com/

CYBERLIPID CENTER

1. This site for cyberlipid studies is an online, non-profit scientific organization whose purpose is to collect, study and diffuse information on all aspects of lipidology.
2. The site seeks to establish contacts between students, teachers, scientists and technicians and expose various models in all fields, forgotten studies of the past, work in progress and hot fields.
3. The site will try to feature an extensive, always upgraded, annotated bibliography devoted to the main presented topics.

Odkazy

[Lipid suppliers]

[Sites directly involved in fat and lipids]

[Journals devoted to lipids]

[General organizations]

[Companies involved in Scientific Research]

[Sites devoted to sciences and techniques]

[Databases and encyclopedia]

[Browsing on the net]

[Discussion Groups]

[Food and Nutrition journals on-line]

[Scientific journals]

[Scientific Societies and organizations]

[Scientific Libraries]

[Publishers]

Historie

1758

First study by Poulletier de la Salle FP of a lipid (cholesterol) isolated from bile stones.

1779

Discovery by the Swedish scientist Scheele CW of glycerol obtained by heating several oils and fats with lead oxide.

1783

Fourcroy AF introduced alcohol to extract brain lipids.

Kalendář

2023

18th-20th January 2023 – Exceptional 'Journées Chevreul 80 years of SFEL', Paris
For information contact : web site

22-23 May 2023 – 3rd International Conference Lipid droplets & Oleosomes, Wageningen, The Netherlands
For information contact : web site

2-5 July 2023 – 15th International Congress Congrès ISSFAL/SFEL, Nantes (France).
For information contact : web site

10-12 July 2023 – 4th EpiLipidNET Action Meeting. Toulouse, France.
For information : web site

17-20 September 2023 – 19th Euro Fed Lipid Congress & Expo, Poznan (Pologne).
For information contact : web site

Lipid classification, structures and tools*

Eoin Fahy*, **Dawn Cotter**, **Manish Sud**, and **Shankar Subramaniam**
University of California, San Diego, 9500 Gilman Dr., La Jolla, CA 92093-0411, USA

Abstract

The study of lipids has developed into a research field of increasing importance as their multiple biological roles in cell biology, physiology and pathology are becoming better understood. The Lipid Metabolites and Pathways Strategy (LIPID MAPS) consortium is actively involved in an integrated approach for the detection, quantitation and pathway reconstruction of lipids and related genes and proteins at a systems-biology level. A key component of this approach is a bioinformatics infrastructure involving a clearly defined classification of lipids, a state-of-the-art database system for molecular species and experimental data and a suite of user-friendly tools to assist lipidomics researchers. Herein, we discuss a number of recent developments by the LIPID MAPS bioinformatics core in pursuit of these objectives. This article is part of a Special Issue entitled Lipodomics and Imaging Mass Spectrometry.

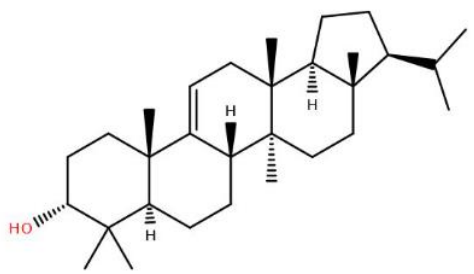
Lipidy a lipidomika

International Lipid Classification and Nomenclature Committee (2005):

Klasifikační systém zahrnující 8 hlavních kategorií, každá je dále členěná (třídy, podtřídy a někdy podpodtřídy)

Lipid of the Month

April, 2023



Arborinol

Lipid Classification System

The LIPID MAPS Lipid Classification System is comprised of eight lipid categories, each with its own subclassification hierarchy. All lipids in the LIPID MAPS Structure Database (LMSD) have been classified using this system and have been assigned LIPID MAPS ID's (LM_ID) which reflects their position in the classification hierarchy. LMSD can be searched by lipid class, common name, systematic name or synonym, mass, InChIKey or LIPID MAPS ID with the search box in the banner, or alternatively, by LIPID MAPS ID, systematic or common name, mass, formula, category, main class, subclass data, or structure or sub-structure with one of the search interfaces in the LMSD database section. Each LMSD record contains an image of the molecular structure, common and systematic names, links to external databases, Wikipedia pages (where available), other annotations and links to structure viewing tools. In addition to LMSD search interfaces, you can drill down through the classification hierarchy below to the LMSD record for an individual lipid.

Lipidy – strukturní databáze

- Třídění lipidů a informatika lipidů obecně je, ve srovnání s proteiny a nukleovými kyselinami, poměrně nový obor.
- LIPID MAPS Structure Database (LMSD)

The LIPID MAPS® Structure Database (LMSD) is a relational database encompassing structures and annotations of biologically relevant lipids. As of today, LMSD contains 47433 unique lipid structures, making it the largest public lipid-only database in the world.

The LIPID MAPS® Structure Database (LMSD) is a relational database encompassing structures and annotations of biologically relevant lipids. As of today, LMSD contains 47877 unique lipid structures, making it the largest public lipid-only database in the world.

https://www.lipidmaps.org/data/structure/index.php

Lipid Category	Curated	Computationally-generated	All
Fatty Acyls [FA]	8676	1878	10554
Glycerolipids [GL]	354	7379	7733
Glycerophospholipids [GP]	1747	8328	10075
Sphingolipids [SP]	1801	3168	4969
Sterol Lipids [ST]	3649	0	3649
Prenol Lipids [PR]	2401	0	2401
Saccharolipids [SL]	51	1294	1345
Polyketides [PK]	7151	0	7151
TOTAL	**25830**	**22047**	**47877**

Structures of lipids in the database come from several sources: (i) LIPID MAPS Consortium's core laboratories and partners; (ii) lipids identified by LIPID MAPS experiments; (iii) biologically relevant lipids manually curated from LIPID BANK, LIPIDAT, Lipid Library, Cyberlipids, ChEBI and other public sources; (iv) novel lipids submitted to peer-reviewed journals; (v) computationally generated structures for appropriate classes.

→ **Klasifikace podle LIPID MAPS systému** → **Přidělení ID**

LIPID ID (LM ID) format

Characters	Position	Description
LMFA01030001	1–2	Database designation
LM**FA**01030001	3–4	Two-letter category code
LMFA**01**030001	5–6	Two-digit class code
LMFA01**03**0001	7–8	Two-digit subclass code
LMFA0103**0001**	9–12	Unique four character identified with in a subclass

Lipidy – strukturní databáze

- Třídění lipidů a informatika lipidů obecně je, ve srovnání s proteiny a nukleovými kyselinami, poměrně nový obor.
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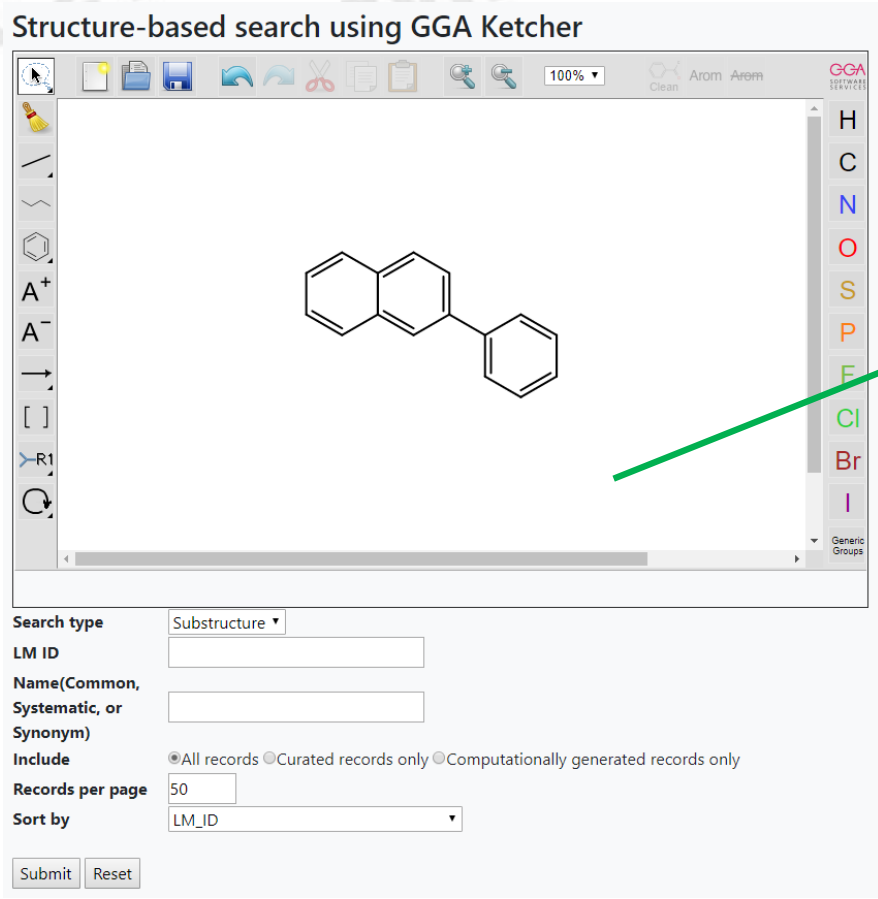
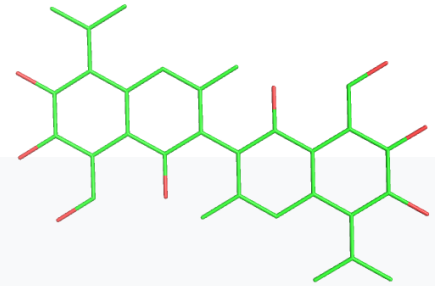
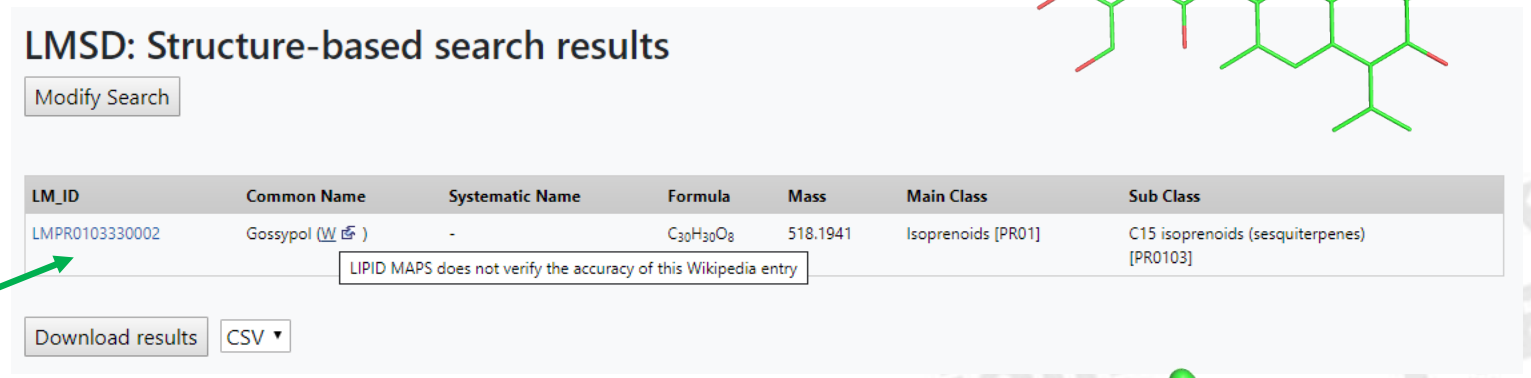
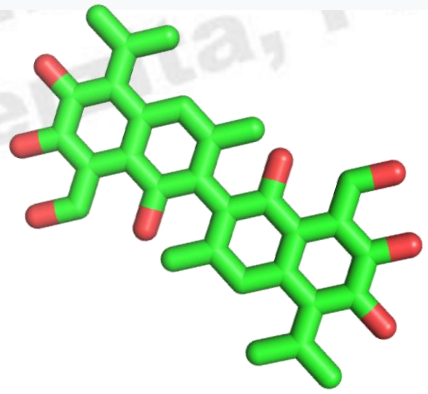
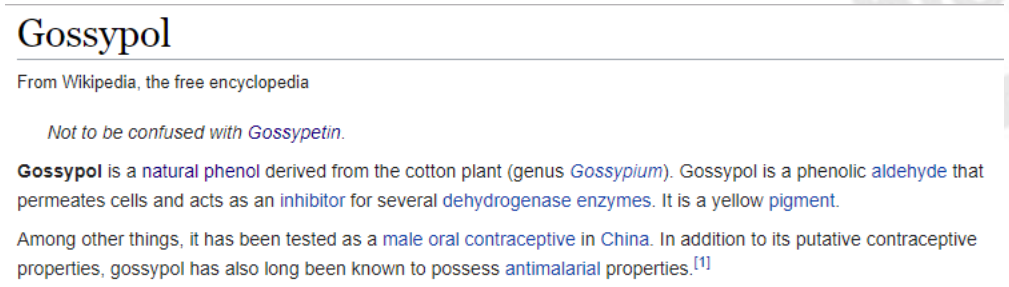








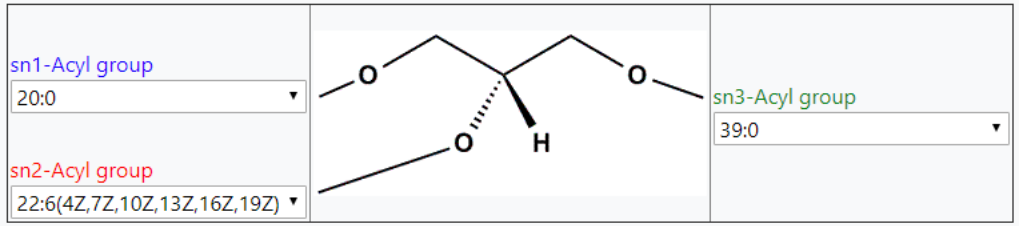


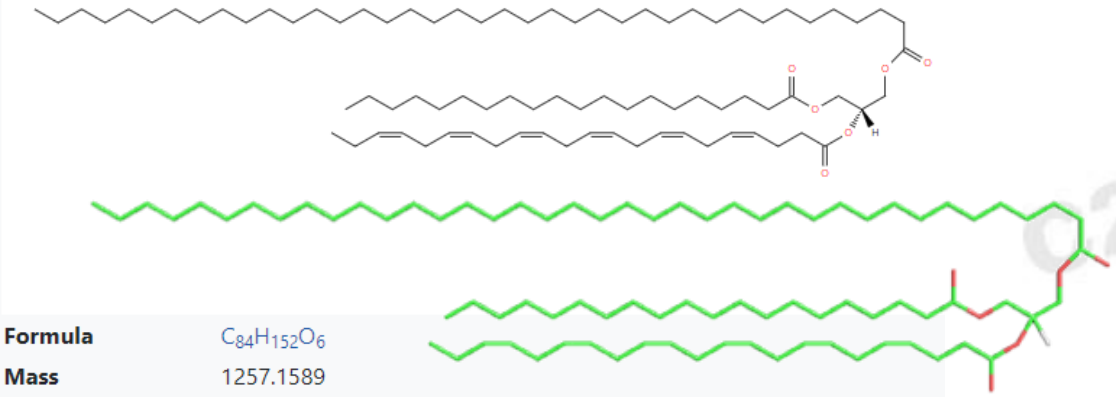
https://www.lipidmaps.org/

(Bio)informatické nástroje

Nástroje pro grafické znázornění lipidů

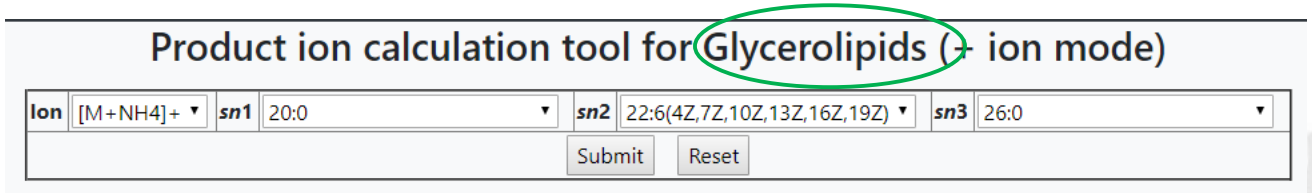
Lipid Structure Drawing Tools





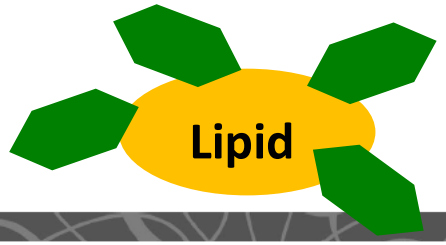
Nástroje pro MS analýzu lipidů

Mass Spectrometry Tools



Commonly occurring product ions for TG(20:0/22:6(4Z,7Z,10Z,13Z,16Z,19Z)/26:0)

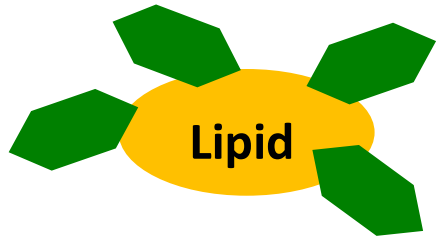
m/z	Ion Description
1092.9893	Precursor ion [M+NH4]+
1075.9627	Precursor ion [M+H]+
1057.9521	Precursor ion [M+H]+ with loss of H2O
763.6599	Neutral loss of sn1 RCOOH + NH3 from [M+NH4]+
747.7225	Neutral loss of sn2 RCOOH + NH3 from [M+NH4]+
679.5660	Neutral loss of sn3 RCOOH + NH3 from [M+NH4]+
453.4302	sn3 acyl chain ([RC=O +74]+)
435.4196	sn3 acyl chain ([RC=O +74]+ with loss of H2O)
385.2737	sn2 acyl chain ([RC=O +74]+)
379.3934	sn3 acyl chain ([RC=O]+)
369.3363	sn1 acyl chain ([RC=O +74]+)
367.2631	sn2 acyl chain ([RC=O +74]+ with loss of H2O)
361.3829	sn3 acyl chain ([RC=O]+ with loss of H2O)
351.3257	sn1 acyl chain ([RC=O +74]+ with loss of H2O)
311.2369	sn2 acyl chain ([RC=O]+)
295.2995	sn1 acyl chain ([RC=O]+)
293.2264	sn2 acyl chain ([RC=O]+ with loss of H2O)
277.2890	sn1 acyl chain ([RC=O]+ with loss of H2O)



Lipidy + sacharidy

- Antigeny
- Receptory
- Adheze

- Lipidová část slouží k ukotvení v membráně



Glycolipids: Animal

Hakomori Sen-itiroh, *Pacific Northwest Research Institute and University of Washington, Seattle, Washington, USA*

Ishizuka Ineo, *Teikyo University School of Medicine, Tokyo, Japan*

Advanced article

Article Contents

Glycolipids are carbohydrates linked to lipid (either ceramide or glyceride). They are found in animal cells and tissues.

doi: 10.1002/9780470015902.a0000706.pub2

Introduction

Glycolipids are ubiquitous components of all animal cell membranes and are particularly abundant at the cell surface membrane. The majority of glycolipids belong to the class 'glycosphingolipids' (GSLs; also called sphingoglycolipids), which have a backbone lipid (termed 'ceramide') consisting of fatty acids and a long-chain aliphatic amino alcohol, discovered and named 'sphingosine' by JLW Thudichum in 1876. Sphingosine has the structure 1,3-dihydroxy-2-amino-octadecene, exhibiting the D-erythro stereoconfiguration with regard to the asymmetric carbon 1 (C1), C2 and C3 (**Figure 1a**). Fatty acids with various chain lengths are linked to the 2-amino group of sphingosine to form ceramide (**Figure 1b**). Various sugar residues are linked to the C1 primary hydroxyl group of the sphingosine moiety in ceramide to form galactosylceramide (GalCer) (**Figure 1c**), glucosylceramide (GlcCer) (**Figure 1d**), or a variety of more complex oligosaccharides, resulting in a wide variety of GSLs. One example of such a structure, 'GM3', which has sialic acid, galactose and glucose, is shown in **Figure 1e**. The sugar linkage to the C1 hydroxyl group of ceramide is always β, with only a single known exception – α-Gal ceramide, which is found in sea anemones.

GSLs are also found in plants, including yeast, although the ceramide and carbohydrate structures are distinctively different from those of animal GSLs. The ceramide of plant GSLs has a sphingosine analogue, termed 'phytosphingosine', which has an additional hydroxyl group at the C4 position. The carbohydrate moiety of plant GSLs has a novel glycan, termed 'phytoglycosphingolipid', consisting of phosphoinositol, glucosamine and mannose. GSLs are rarely found in bacteria, except for a novel group of 'sphingobacteria' that includes *Sphingomonas paucimobilis*.

A further class of glycolipids, termed 'glycoglycerolipids', has been found and characterized. They have 1,2-diacyl-*sn*-glycerol or 1–alkyl-2-acyl-*sn*-glycerol as a backbone lipid, to which a monosaccharide or relatively short oligosaccharide is linked through the primary hydroxyl group (**Figure 2**). Only two glycoglycerolipids have been well characterized as animal tissue components. Their distribution is limited to the nervous system (brain, spinal cord, peripheral nerves) and testis. In contrast to animal tissues, glycoglycerolipids are the major component in plants and bacteria.

Another class of glyceroglycolipids is the 'glycosylphosphatidylinositol anchor' (GPI anchor). A large number of functionally important cell-surface proteins are anchored through this class of glycoglycerolipids (see below). **See also**: Glycolipids: distribution and biological function

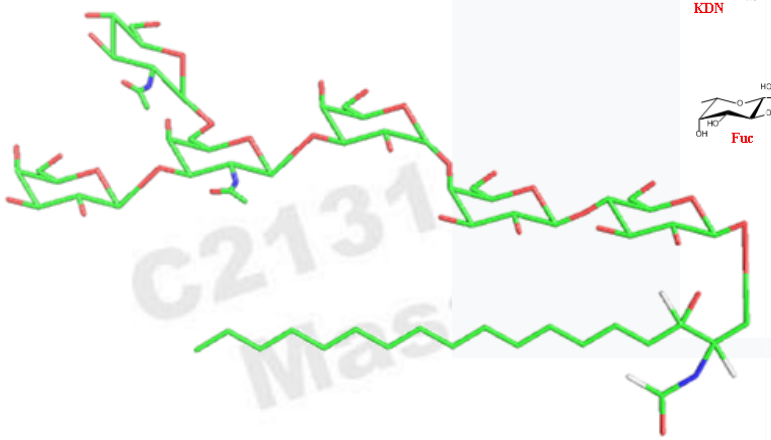
Structure

The most extensive studies on the structure and function of animal cell glycolipids have been focused on GSLs. GSLs consist of two distinct moieties: ceramide, which is hydrophobic, and carbohydrate, which is hydrophilic. A molecular model of GSL based on X-ray crystallography indicates that the axis of the ceramide is perpendicular to the axis of the carbohydrate chain. GSLs have a strong tendency to aggregate to form micelles in aqueous media, or to form microdomains in the cell membrane bilayer.

GSLs from animal tissues are classified according to two criteria: (1) the presence or absence of strongly acidic group (sialic acid or sulfate), or cationic amino group (very rarely present); and (2) differences in core carbohydrate structure. Four subclasses based on criterion (1) are neutral GSLs, gangliosides (GSLs containing sialic acid), sulfatide (sulfated GSL) and a few cationic GSLs having free amino group. Three subclasses based on criterion (2) are: ganglio-series, lacto-series and globo-series GSLs. In the current literature, approximately 50 ganglio-series, 80 lacto-series and 10 globo-series GSLs are known. For ganglio-series GSLs, 2 neutral, 7 sulfated and ~40 sialylated species are known. For lacto-series, 14 neutral, 2 sulfated, ~30 sialylated and ~32 fucosylated species are known. In some cases, hybrid types between the lacto- and ganglio-series or between the globo- and lacto-series have been observed. In certain protozoa, parasites and marine invertebrates, novel GSL structures have been observed that cannot be assigned to any of the three subclasses described above.

Neutral glycosphingolipids

The most abundant GSL in animal tissues is galactosylceramide (GalCer; cerebroside) in brain, discovered by



Create a Sphingolipid Glycan Structure

https://www.lipidmaps.org/

Core: Ceramide

Core chain style: Straight

Glycan: Galb1-3(GlcNAcb1-6)GalNAcb1-3Gala1-4Galb1-4Glcb

Glycan chain orientation: Left

Submit Reset

Usage

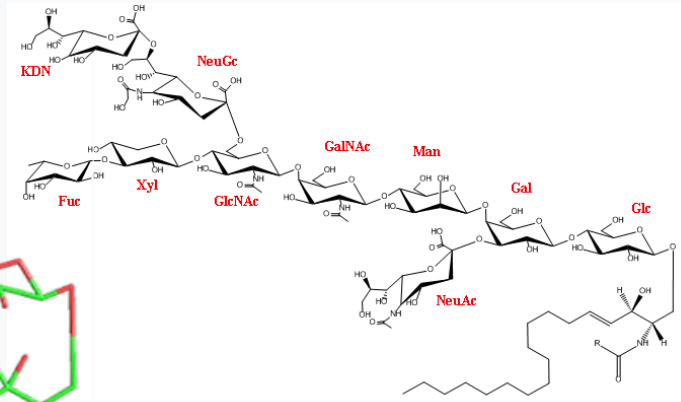
Sugar residues allowed: **Glc, Gal, Man, GlcNAc, GalNAc, Xyl, Fuc, NeuAc, NeuGc, KDN**

Glycan sequence must be in the format: **[sugar (as an abbreviation)][anomer (either a or b)][linkage in (x-y form)]**

Examples: Galb1-4Glcb, Fuca1-2Galb1-3GalNAcb1-4Galb1-4Glcb, NeuAca2-3Galb1-3GalNAcb1-3Gala1-4Galb1-4Glcb

Branched glycans are designated by parentheses: GalNAca1-3GalNAcb1-3(Galb1-3GalNAcb1-4)Gala1-4Galb1-4Glcb

(The hypothetical structure below contains all 10 sugar residues currently supported)



Lipidy + proteiny

LipoP - 1.0

Signal peptidase I & II cleavage sites in gram- bacteria

The LipoP 1.0 server produces predictions of lipoproteins and discriminates between lipoprotein signal peptides, other signal peptides and n-terminal membrane helices in Gram-negative bacteria.

Note: Although LipoP 1.0 has been trained on sequences from Gram-negative bacteria only, the following paper reports that it has a good performance on sequences from Gram-positive bacteria also:

Methods for the bioinformatic identification of bacterial lipoproteins encoded in the genomes of Gram-positive bacteria
O. Rahman, S. P. Cummings, D. J. Harrington and I. C. Sutcliffe
World Journal of Microbiology and Biotechnology **24**(11):2377-2382 (2008)

https://services.healthtech.dtu.dk/service.php?LipoP-1.0

NOTE: LipoP is outdated and is only kept online for reference. Lipoprotein signal peptides are better predicted by the current version of SignalP!

MINIREVIEWS

Lipoproteins of Bacterial Pathogens[▽]

A. Kovacs-Simon, R. W. Titball, and S. L. Michell*

Abstract Bacterial lipoproteins are a diverse and functionally important group of proteins that are amenable to bioinformatic analyses because of their unique signal peptide features. Here we have used a dataset of sequences of experimentally verified lipoproteins of Gram-positive bacteria to refine our previously described lipoprotein recognition pattern (G+LPP). Sequenced bacterial genomes can be screened for putative lipoproteins using the G+LPP pattern. The sequences identified can then be validated using online tools for lipoprotein sequence identification. We have used our protein sequence datasets to evaluate six online tools for efficacy of lipoprotein sequence identification. Our analyses demonstrate that LipoP (http://www.cbs.dtu.dk/services/LipoP/) performs best individually but that a consensus approach, incorporating outputs from predictors of general signal peptide properties, is most informative.

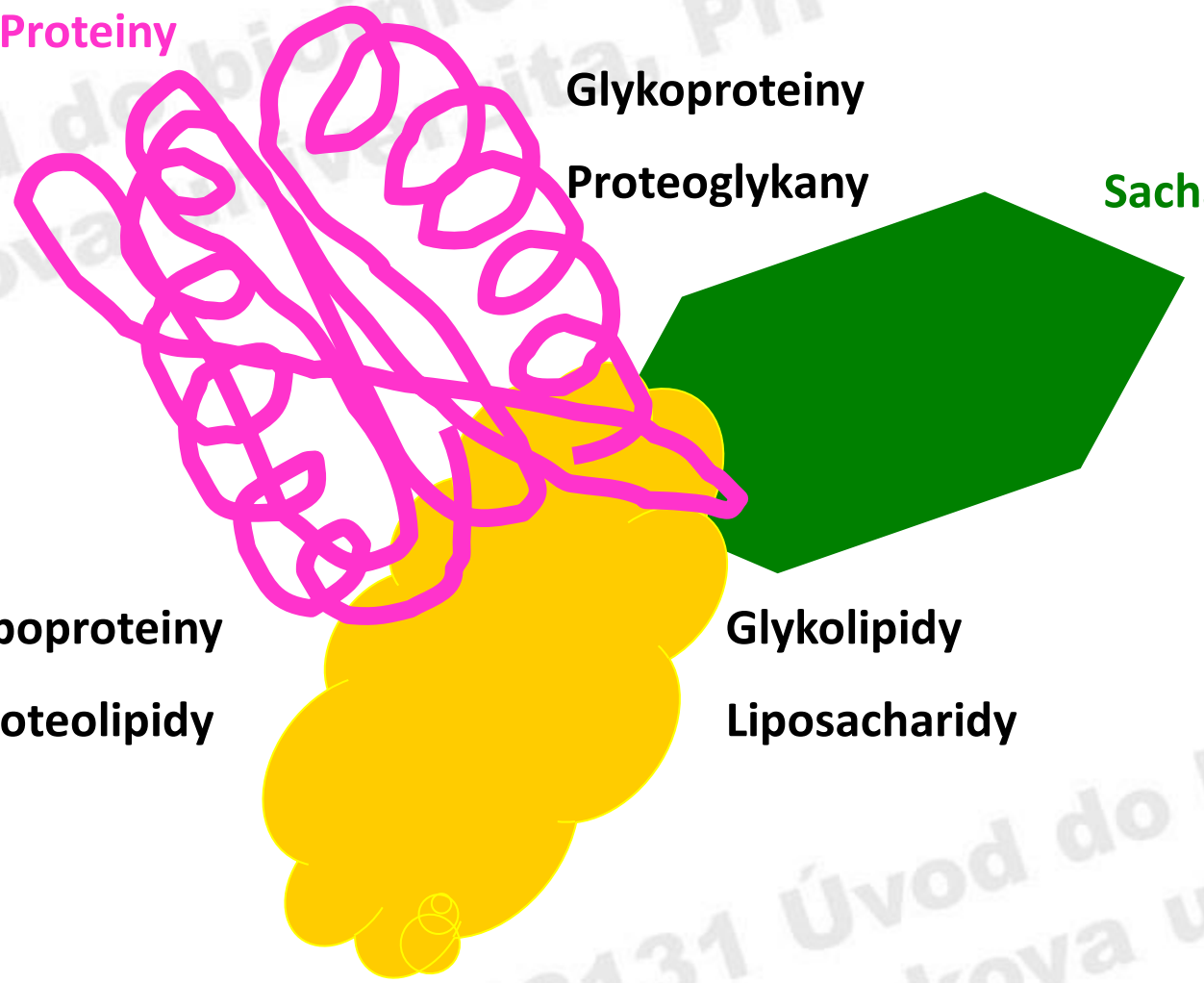
SignalP - 6.0

Prediction of Signal Peptides and their cleavage sites in all domains of life

The SignalP 6.0 server predicts the presence of signal peptides and the location of their cleavage sites in proteins from Archaea, Gram-positive Bacteria, Gram-negative Bacteria and Eukarya. In Bacteria and Archaea, SignalP 6.0 can discriminate between five types of signal peptides:

Sec/SPI: "standard" secretory signal peptides transported by the Sec translocon and cleaved by Signal Peptidase I (*Lep*)
Sec/SPII: lipoprotein signal peptides transported by the Sec translocon and cleaved by Signal Peptidase II (*Lsp*)
Tat/SPI: Tat signal peptides transported by the Tat translocon and cleaved by Signal Peptidase I (*Lep*)
Tat/SPII: Tat lipoprotein signal peptides transported by the Tat translocon and cleaved by Signal Peptidase II (*Lsp*)
Sec/SPIII: Pilin and pilin-like signal peptides transported by the Sec translocon and cleaved by Signal Peptidase III (*PilD/PibD*)

https://services.healthtech.dtu.dk/services/SignalP-6.0/



Všechno souvisí se vším…

C2131 Úvod do bioinformatiky
Masarykova univerzita, PřF

„Take-home message“

- **Sacharidy: zdroj/zásoba energie, stavební a informační funkce.**
- **Na syntéze komplexních glykanů se podílí množství proteinů (genů).**
- **Glykosylace je významná posttranslační modifikace (funkce x poruchy x predikce).**
- **Lektiny – proteiny, které specificky a reverzibilně vážou sacharidy.**
- **Na rozdíl od NA/proteinů se u sacharidů často používá grafické znázornění.**
- **Výpočetní nástroje jsou důležité i pro zpracování experimentálních dat.**
- **Lipidy nejsou jen zdroj/zásoba energie ☺**

Použitá a doporučená literatura

Terminology of bioanalytical methods (IUPAC Recommendations 2018)

https://doi.org/10.1515/pac-2016-1120
Received November 21, 2016; accepted February 1, 2018

Evolutionary aspects of ABO blood group in humans

Massimo Franchini *, Carlo Bonfanti

Department of Hematology and Transfusion Medicine, Azienda Ospedaliera Carlo Poma, Mantova, Italy

ABSTRACT

The antigens of the ABO blood group system (A, B and H determinants) are complex carbohydrate molecules expressed on red blood cells and on a variety of other cell lines and tissues. Growing evidence is accumulating that ABO antigens, beyond their key role in transfusion medicine, may interplay with the pathogenesis of many human disorders, including infectious, cardiovascular and neoplastic diseases. In this narrative review, after succinct description of the current knowledge on the association between ABO blood groups and the most severe diseases, we aim to elucidate the particularly intriguing issue of the possible role of ABO system in successful aging. In particular, focus will be placed on studies evaluating the ABO phenotype in centenarians, the best human model of longevity.

Lectins

Nathan Sharon, *Weizmann Institute of Science, Rehovot, Israel*

Based in large part on the previous version of this Encyclopedia of Life Sciences (ELS) article, Lectins by Nathan Sharon and Halina Lis.

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Advanced Drug Delivery Reviews 56 (2004) 425–435

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Lectin-mediated drug targeting: history and applications

Christiane Bies[a], Claus-Michael Lehr[a], John F. Woodley[b,*]

[a] *Department of Biopharmaceutics and Pharmaceutical Technology, Saarland University, Saarbrücken, Germany*
[b] *Laboratoire de Cinétique des Xénobiotiques, Faculté des Sciences Pharmaceutiques, 35 chemin des Maraîchers, 31062 Toulouse, France*

Received 8 October 2003; accepted 14 October 2003

Chem Soc Rev

RSC Publishing

REVIEW ARTICLE

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Cite this: *Chem. Soc. Rev.*, 2013, **42**, 4709

Multivalent glycoconjugates as anti-pathogenic agents†

Anna Bernardi,[a] Jesus Jiménez-Barbero,[b] Alessandro Casnati,[c] Cristina De Castro,[d] Tamis Darbre,[e] Franck Fieschi,[f] Jukka Finne,[g] Horst Funken,[h] Karl-Erich Jaeger,[h] Martina Lahmann,[i] Thisbe K. Lindhorst,[j] Marco Marradi,[k] Paul Messner,[l] Antonio Molinaro,[d] Paul V. Murphy,[m] Cristina Nativi,[n] Stefan Oscarson,[o] Soledad Penadés,[k] Francesco Peri,[p] Roland J. Pieters,[q] Olivier Renaudet,[r] Jean-Louis Reymond,[e] Barbara Richichi,[n] Javier Rojo,[s] Francesco Sansone,[c] Christina Schäffer,[l] W. Bruce Turnbull,[t] Trinidad Velasco-Torrijos,[u] Sébastien Vidal,[v] Stéphane Vincent,[w] Tom Wennekes,[x] Han Zuilhof[xy] and Anne Imberty*[z]

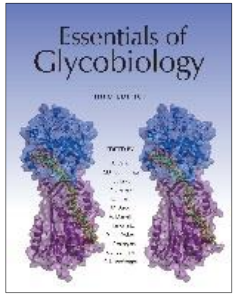
Glycoconj J (2013) 30:41–50
DOI 10.1007/s10719-012-9397-y

Genomics and epigenomics of the human glycome

Vlatka Zoldoš · Mislav Novokmet · Ivona Bečeheli · Gordan Lauc

New insights into influenza A specificity: an evolution of paradigms

Ye Ji, Yohanna JB White, Jodi A Hadden[1], Oliver C Grant and Robert J Woods



Technical Note

SugarSketcher: Quick and Intuitive Online Glycan Drawing

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Proteomics 2013, *13*, 341–354 DOI 10.1002/pmic.201200149

Host cell recognition by the henipaviruses: Crystal structures of the Nipah G attachment glycoprotein and its complex with ephrin-B3

Kai Xu*, Kanagalaghatta R. Rajashankar†, Yee-Peng Chan‡, Juha P. Himanen*, Christopher C. Broder‡, and Dimitar B. Nikolov*§

*Structural Biology Program, Memorial Sloan–Kettering Cancer Center, 1275 York Avenue, New York, NY 10021; †Northeastern Collaborative Access T

Použitá a doporučená literatura

Glycoproteins

Tony Merry, *University of Manchester, Manchester, UK*
Sviatlana Astrautsova, *Grodno State Medical University, Grodno, Belarus*

Based in part on the previous version of this Encyclopedia of Life Sciences (ELS) article, "Glycoproteins" by "Terry D Butters".

Glycolipids: Animal

Hakomori Sen-itiroh, *Pacific Northwest Research Institute and University of Washington, Seattle, Washington, USA*
Ishizuka Ineo, *Teikyo University School of Medicine, Tokyo, Japan*

Glycolipids are carbohydrates linked to lipid (either ceramide or glyceride). They are found in animal cells and tissues.

Advanced article

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- Structure
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Eoin Fahy[*], **Dawn Cotter**, **Manish Sud**, and **Shankar Subramaniam**
University of California, San Diego, 9500 Gilman Dr., La Jolla, CA 92093-0411, USA

MINIREVIEWS

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A. Kovacs-Simon, R. W. Titball, and S. L. Michell*

Kazuistika dívky s dědičnou poruchou glykosylace

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Klinika dětského a dorostového lékařství, 1. LF UK a VFN Praha

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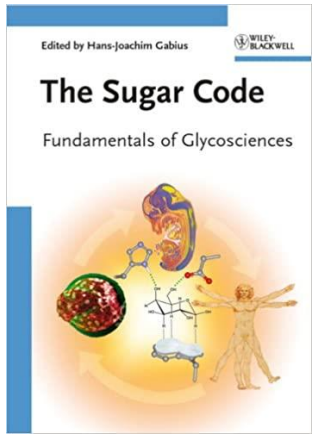

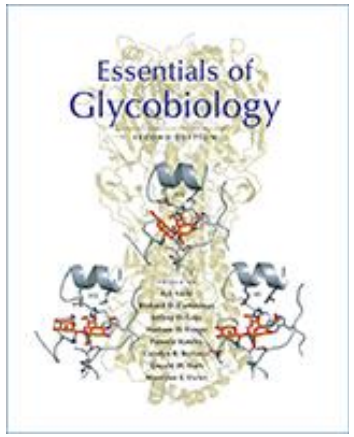

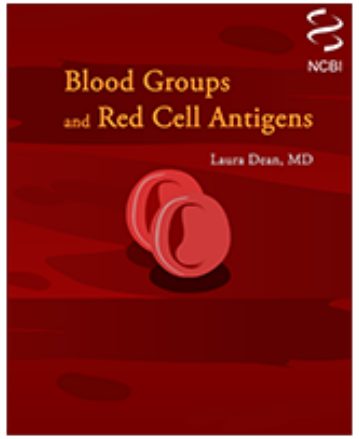

Lipidomics: a global approach to lipid analysis in biological systems

Andrew D. Watson[1]
Department of Medicine, Division of Cardiology, David Geffen School of Medicine, University of California at Los Angeles, Los Angeles, CA 90095

554 Review *TRENDS in Microbiology* Vol.11 No.12 December 2003

Sweet new world: glycoproteins in bacterial pathogens

M. Alexander Schmidt[1], **Lee W. Riley**[2] **and Inga Benz**[1]
[1]Institut für Infektiologie, Zentrum für Molekularbiologie der Entzündung (ZMBE), Von-Esmarch-Str. 56, D-48149 Münster, Germany
[2]Division of Infectious Diseases and Immunity, School of Public Health, University of California, 140 Warren Hall, Berkeley, CA 94720, USA